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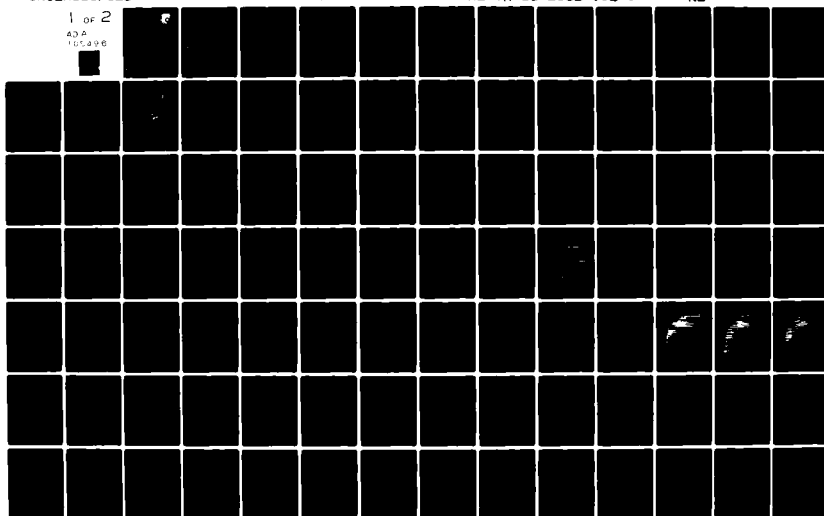
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INVESTIGATION OF PLASMA EXCITATION  
Volume III: Advanced Optical Diagnostics

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C. A. DeJoseph  
Universal Energy Systems, Inc.  
3195 Plainfield Road  
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August 1981

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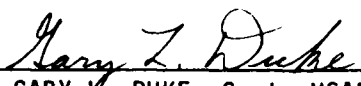
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A Fourier transform infrared spectrometer was used to identify infrared absorption spectra of impurities that might be present in CO <sub>2</sub> laser discharges. Spectral regions free from interference from the primary constituents and common impurities such as water vapor were identified for several of the nitrogen oxides, and the detection sensitivities were determined. This infor- mation was used in a study of impurity buildup during discharges in an electron-beam excited closed cycle (EBCC) system and in a TEA CO <sub>2</sub> laser.		

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It was found that after an hour of irradiation in the continuous EBCC system, the oxides of nitrogen had built up to the ten parts per million range while the carbon monoxide concentration was of the order of a few hundred parts per million. When the initial gas mix contained oxygen, the concentration of ~~CO~~ and the nitrogen oxides increased. The addition of hydrogen to an oxygen free gas mix was found to produce water vapor at about ten percent of the initial hydrogen concentration, increase the production of  $N_2O$  and of  $CO$ , and decrease the production of  $NO$  and  $NO_2$ .

A technique has been developed for determining the rotational temperature and vibrational population distribution of non-homonuclear molecules under nonequilibrium conditions. The technique was applied to carbon monoxide under the conditions present in an electrical discharge.

*carbon monoxide*

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## FOREWORD

This report describes research performed by Universal Energy Systems, Inc., Dayton, Ohio. The work was conducted under Contract F33615-77-C-3113, "Investigations of Methods of Plasma Excitation," Task III, "Advanced Optical Diagnostics of Plasmas."

The work reported herein was performed at in-house facilities of the Air Force Aero Propulsion Laboratory, Air Force Wright Aeronautical Laboratories, Wright-Patterson Air Force Base, Ohio. The experimental work and analysis described was performed by C. A. DeJoseph. As Mr. DeJoseph was not employed by Universal Energy Systems at the time of the completion of the contract, this section of the final report was prepared by V. E. Merchant by combining and editing quarterly reports previously written by Mr. DeJoseph.

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## SECTION I

### INTRODUCTION

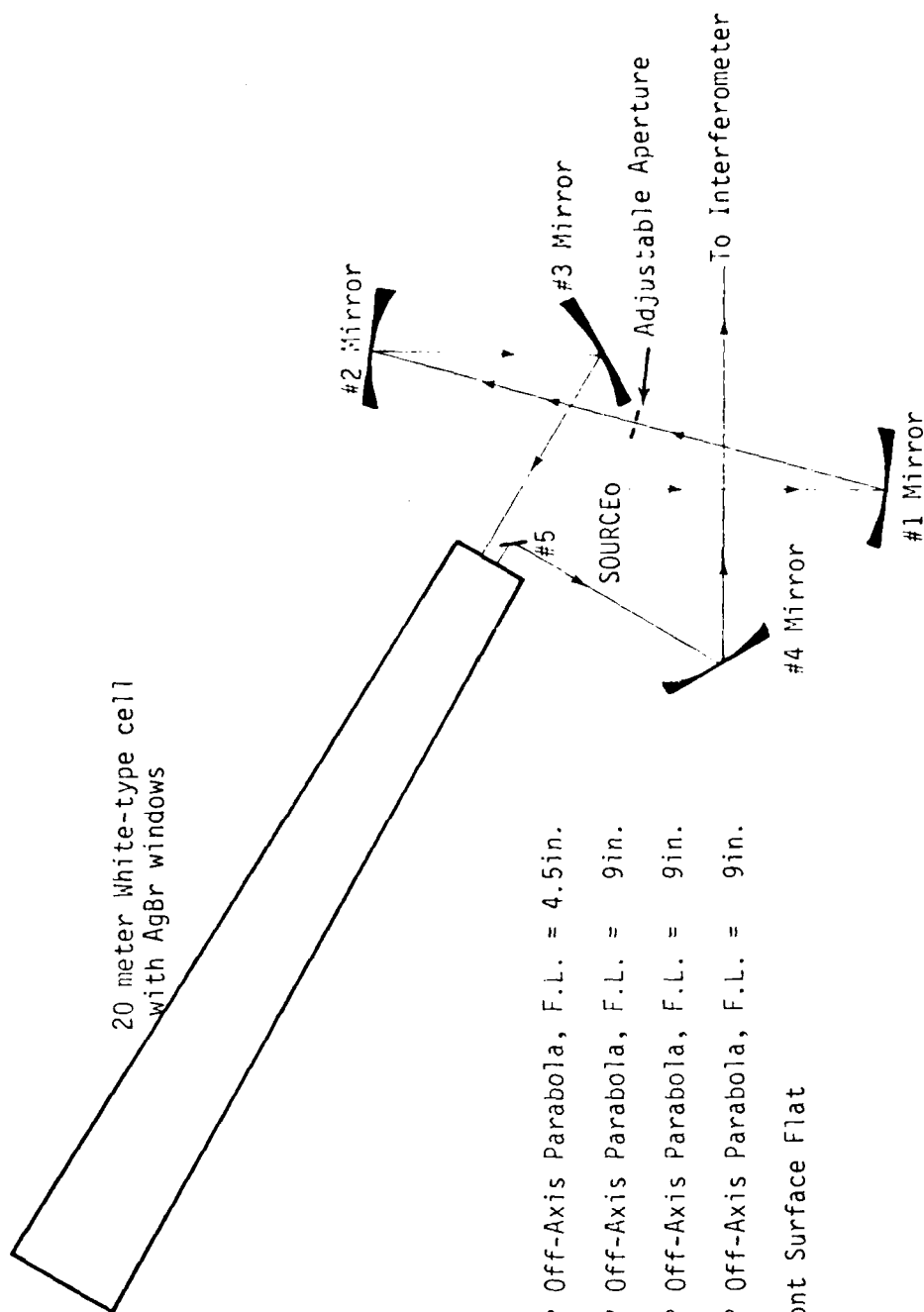
Advanced optical techniques have been applied to several problems in plasmas diagnostics. A technique has been developed for determining the rotational temperature and vibrational population distribution of non-homonuclear molecules under non-equilibrium conditions. The technique was applied to carbon monoxide under the conditions present in an electrical discharge. The second problem area was identifying infrared absorption spectra of impurities that might be present in CO<sub>2</sub> laser discharges. Spectral regions free from interference from the primary constituents and common impurities such as water vapor were identified for several of the nitrogen oxides, and the detection sensitivities were determined. Finally this information was used in a study of impurity buildup during discharges in an electron-beam excited closed cycle (EBCC) system and in a TEA laser.

Succeeding sections of this report give more information about the developments in these main areas of concentration. In addition several minor problems were addressed. The infrared transmittance of Freon 1301 in the 10.6  $\mu\text{m}$  spectral region was investigated. Infrared emission spectra were obtained from He-Ne and He-Xe hollow cathode discharges. No further information about these minor problem areas will be given here.

Throughout the duration of the contract, several improvements were made to the Fourier Transform Spectrometer (FTS). A variable path corrosion resistant absorption cell and associated gas handling hardware were added to the system for use with corrosive gases. The system constructed for the trace species absorption measurements is centered around a long-path (20 meters) White-type infrared absorption cell with optics for use with the FTS system.

In addition, a stainless steel, high vacuum gas handling system is used for evacuating the cell and preparing the synthetic mixes. Figure 1 shows the layout of the optics system for the White cell. The glowbar source is imaged 1:1 onto the adjustable aperture by mirror #1 and then collimated by mirror #2. Mirror #3 focuses the radiation onto the entrance window of the White cell and the radiation leaving the cell is re-collimated by mirror #4. Radiation leaving mirror #4 then passes to the FTS System where the spectrum is measured. Figure 2 shows the gas handling system for the White cell. High vacuum evacuation of the system is by the liquid nitrogen trapped diffusion pump. Base pressure for the system is the mid  $10^{-7}$  torr range. The system can be used in two ways. Samples of gas from the EBCC loop can be entered into the system via the sample port or absorption spectra of various gas mixes can be obtained by entering these into the system through the gas manifold. Gas pressure was measured with the two MKS Baratron which gave an increase in dynamic range of pressure measurement over a single unit. Gas mixes were prepared under static pressure conditions and likewise the absorption measurements were made under static conditions. After a gas fill, the White cell was "roughed down" using forepump #2 which is a high throughput Leybold Heraeus model DK-45. Use of this pump greatly facilitated pump down of the cell from atmospheric pressure while allowing forepump #1 to remain small for reduced backstreaming to the diffusion pump.

The spectral range of study was originally limited to the range of  $5.9 \mu\text{m}$  to  $1.7 \mu\text{m}$  ( $1700\text{-}6000 \text{ cm}^{-1}$ ). This is the range over which the original PbSe detector used in the FTS System was sensitive. A new "sandwich" detector was obtained which allowed the range to be extended from  $14 \mu\text{m}$  to  $1.7 \mu\text{m}$  ( $700\text{-}6000 \text{ cm}^{-1}$ ). This detector is composed of a  $\text{LN}_2$  cooled HgCdTe detector "sandwiched" behind a  $\text{LN}_2$  cooled InSb detector. The detector



- #1 Mirror: 15° Off-Axis Parabola, F.L. = 4.5 in.
- #2 Mirror: 15° Off-Axis Parabola, F.L. = 9 in.
- #3 Mirror: 60° Off-Axis Parabola, F.L. = 9 in.
- #4 Mirror: 60° Off-Axis Parabola, F.L. = 9 in.
- #5 Mirror: Front Surface Flat

FIGURE 1 WHITE-CELL OPTICS

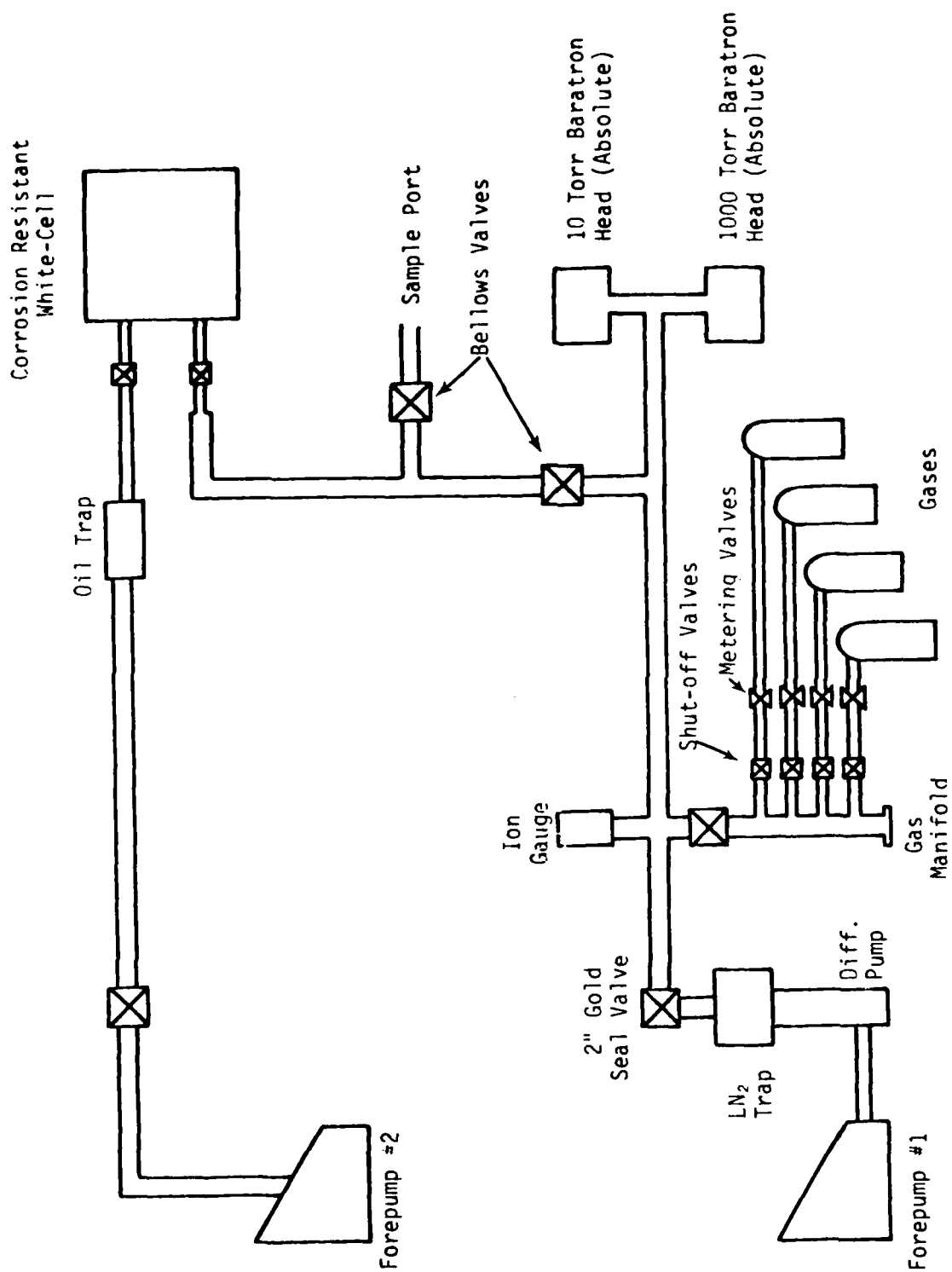


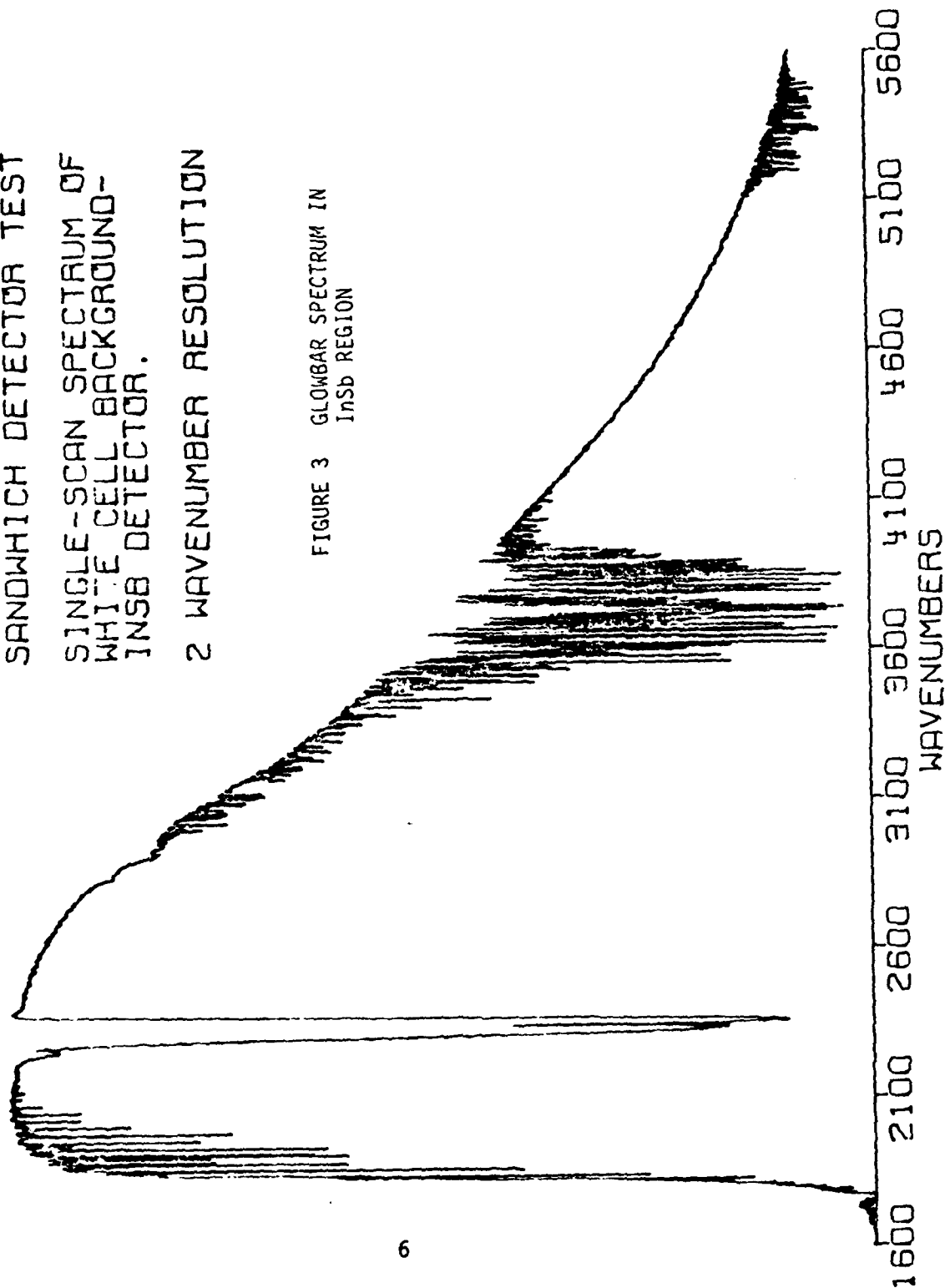
FIGURE 2 WHITE-CELL GAS HANDLING SYSTEM

can be wired so that the outputs are added or come out separately, with each configuration having its own advantages and disadvantages. For maximum signal-to-noise, the outputs are taken separately and either part of the composite detector is selected by the FTS System controller. Thus, in its present configuration the FTS System can gather data in the range of the HgCdTe detector, ie.  $14\text{ }\mu\text{m}$  to  $5.4\text{ }\mu\text{m}$  ( $700\text{--}1850\text{ cm}^{-1}$ ) or the InSb detector, ie.  $5.7\text{ }\mu\text{m}$  to  $1.7\text{ }\mu\text{m}$  ( $1750\text{--}6000\text{ cm}^{-1}$ ). Results shown in this report were primarily obtained with the PbSe detector. Most measurements were taken in the presence of laboratory air, so it was necessary to contend with parasitic absorption by water vapor and carbon dioxide in the air. Figure 3 shows a low resolution spectrum of the glowbar source as seen through the White cell in the InSb (or roughly the PbSe) region of the spectrum in lab air. The regions showing absorption due to  $\text{H}_2\text{O}$  and  $\text{CO}_2$  must be taken into account when deciding where to look for absorption by the minor species. Figure 3 will serve to locate absorption features shown in more detailed spectra later in the report.

A significant change to the absorption cell-FTS optics was the installing of a germanium on potassium bromide (KBr) beamsplitter in the FTS system. With this beamsplitter and the "sandwich" detector spectral coverage of the FTS system has been extended to the range  $14\text{ }\mu\text{m}$  to  $2\text{ }\mu\text{m}$ . Because of the way the "sandwich" detector is wired, the spectral range must be covered in two separate data acquisitions. Data is acquired over the spectral range  $14\text{ }\mu\text{m}$  to  $5.4\text{ }\mu\text{m}$  ( $700\text{--}1850\text{ cm}^{-1}$ ) or  $5.7\text{ }\mu\text{m}$  to  $2\text{ }\mu\text{m}$  ( $1750\text{--}5000\text{ cm}^{-1}$ ). Thus, analysis of a gas sample requires two data acquisitions each requiring about twenty minutes to complete. Replacing the iron oxide on calcium flouride ( $\text{CaF}_2$ ) beamsplitter with the KBr extends the spectral region from about  $1100\text{ cm}^{-1}$  to  $700\text{ cm}^{-1}$  on the low frequency side while shortening the region from

SANDWICH DETECTOR TEST  
SINGLE-SCAN SPECTRUM OF  
WHITE CELL BACKGROUND-  
INSB DETECTOR.  
2 WAVENUMBER RESOLUTION

FIGURE 3 GLOWBAR SPECTRUM IN  
InSb REGION





6000  $\text{cm}^{-1}$  to 5000  $\text{cm}^{-1}$  on the high frequency side. However, due to the importance of the 10  $\mu\text{m}$  spectral region in some experiments, the increased coverage in the low frequency part of the spectrum is a more desirable configuration.

An investigation was made of the factors limiting the precision of wavelength determination with the Fourier Transform Spectrometer. The precision with which a line position can be determined is dependent on a number of experimental parameters. One parameter that is fundamental to the best achievable precision is the resolution of the instrument [2]. If the only factor affecting the precision of the measurement is the experimenters ability to locate the center of the line, then the best precision achievable is likely to be between one-twentieth and one-thirtieth of the resolution [2]. The AFAPL FTS system possesses a maximum resolution of 0.6  $\text{cm}^{-1}$  (apodized) and a theoretical resolution of .037  $\text{cm}^{-1}$  (unapodized). Therefore, the maximum precision with which a line position can be determined with this instrument should be on the order of  $\pm .001$  and  $\pm .003 \text{ cm}^{-1}$ . A study was undertaken to determine how closely this maximum could be approached. Wave-number precision of the recovered spectrum from the FTS system is directly dependent on the precision with which the moving mirror position is measured in the interferogram. The mirror position is determined by monitoring the interference fringes produced by a helium-neon (HeNe) laser, so the wave-number scale in the recovered spectrum is reasonably precise due to this technique of mirror position measurement. This "automatic" calibration of the FTS-produced spectrum is sometimes referred to as Conne's advantage.

A number of factors effect the best achievable precision of this "automatic" calibration scheme so an attempt was made to identify and eliminate the largest of these. One factor effecting the precision of the calculated

wavenumbers which is well known is the degree to which radiation from the source is collimated [2]. The reason for this is that rays entering the interferometer off-axis travel a greater distance than those entering on-axis, thus the computed spectrum for the off-axis rays differs from the spectrum computed for on-axis rays. As Bell has shown [2], if the source subtends a solid angle  $\Omega$ , the computed wavenumbers  $\sigma_c$  are related to the true wavenumbers  $\sigma_0$  by;

$$\sigma_c = \sigma_0 (1 - \Omega/4\pi). \quad (1)$$

Thus, a measured line position will be lower in wavenumber than the true line position. Using the small angle approximation for  $\Omega$ , equation (1) can be written,

$$\sigma_c = \sigma_0 (1 - \alpha^2/4)$$

where  $\alpha$  is the angle of deviation of rays entering the interferometer. For example, if one requires the wavenumbers to be within  $\pm 0.01 \text{ cm}^{-1}$  at  $4000 \text{ cm}^{-1}$ ,  $\alpha$  must be 3.2 mrad. or 11 minutes of arc. Thus it is necessary when doing precision line position measurements to precisely control the degree of collimation of the source.

A second source of error results from the apparatus operating in air and the dispersion in the index of refraction of the air. Since the mirror position is measured with the HeNe laser, the wavelength of the laser serves the same purpose as a known line in a conventional spectrometer. Because the known line in the FTS system is quite removed in wavenumber from the unknown lines, the vacuum correction for the HeNe laser is not the proper correction for the IR region of the spectrum. To see this source of error more clearly, consider the fundamental equations of FT-IR. Let the fluctuating part of the interferogram as a function of path difference  $x$  be  $I(x)$ , and

the spectral distribution function be  $B(\sigma)$ . Then for an ideal interferometer,  $I(x)$  and  $B(\sigma)$  are related by, ,

$$I(x) = 2 \int_0^{\infty} B(\sigma) \cos(2\pi\sigma x) d\sigma \quad (2)$$

$$B(\sigma) = 2 \int_0^{\infty} I(x) \cos(2\pi\sigma x) dx \quad (3)$$

where  $\sigma$  is in  $\text{cm}^{-1}$ , and the constant 2 is somewhat arbitrary. Assume that a source possesses a spectral distribution function (in air) of  $B_0(\sigma_0)$ . The measured interferogram from the source,  $I_m(X_m)$ , is then given by,

$$I_m(X_m) = 2 \int_0^{\infty} B_0(\sigma_0) \cos 2\pi\sigma_0 X_m d\sigma_0. \quad (4)$$

The calculated spectrum  $B_c(\sigma_c)$  is given by,

$$B_c(\sigma_c) = 2 \int_0^{\infty} I_m(X_m) \cos 2\pi\sigma_c X_m dX_m. \quad (5)$$

Substituting equation (4) into (5) gives,

$$B_c(\sigma_c) = 4 \int_0^{\infty} \left[ \int_0^{\infty} B_0(\sigma_0) \cos 2\pi\sigma_0 X_m d\sigma_0 \right] \cos 2\pi\sigma_c X_m dX_m. \quad (6)$$

Here the subscripts 'c' and 'm' refer to quantities either used in or the results of calculations, and quantities actually measured. The measured interferogram,  $I_m$ , is acquired by monitoring the fringes of the HeNe laser and sampling at every  $j^{\text{th}}$  zero-crossing of the laser interferogram. The laser interferogram is roughly a cosine wave which crosses zero at  $X = j\lambda/2$  where  $\lambda = \text{HeNe}$  and  $j = 1, 2, 3, \dots$ . Since the laser operates in air, the measured path difference  $X_m$  is sampled with a spacing of  $\Delta X_m$  given by,

$$\Delta X_m = j \cdot \frac{1}{2} \lambda_{\text{Air}}(\text{HeNe}), j = 1, 2, \dots \quad (7)$$

where  $\lambda_{\text{Air}}$  is the wavelength of the helium-neon laser in air. In the calculation of  $B_c(\sigma_c)$ , it is assumed that the path difference was sampled

with a spacing  $\Delta X_c$  given by,

$$\Delta X_c = j \cdot \frac{1}{2} \lambda_{vac}(\text{HeNe}), j = 1, 2, \dots \quad (8)$$

where  $\lambda_{vac}(\text{HeNe})$  is the wavelength of the helium-neon laser in vacuum.

Therefore, in equation (6),  $X_c$  can be written in terms of  $X_m$ , using equations (7) and (8), as

$$X_c = \frac{\lambda_{vac}(\text{HeNe})}{\lambda_{Air}(\text{HeNe})} \cdot X_m \quad (9)$$

In equation (9) the ratio of  $\lambda_{vac}/\lambda_{Air}$  is just the index of refraction of air at the HeNe laser wavelength. So equation (9) becomes

$$X_c = n(\text{HeNe}) \cdot X_m \quad (10)$$

where  $n(\text{HeNe})$  is the index of air. Using equation (10) and letting  $X_m = X_c/n(\text{HeNe})$  in equation (6) gives for the calculated spectrum,

$$B_c(\sigma_c) = 4 \cdot \int_0^\infty \left[ \int_0^\infty B_o(\sigma_o) \cos 2\pi\sigma_o \frac{X_c}{n(\text{HeNe})} d\sigma_o \right] \cos 2\pi\sigma_c X_c dX_c$$

and changing the order of integration gives,

$$B_c(\sigma_c) = 4 \cdot \int_0^\infty B_o(\sigma_o) \left[ \int_0^\infty \cos 2\pi\sigma_o \frac{X_c}{n(\text{HeNe})} \cos 2\pi\sigma_c X_c dX_c \right] d\sigma_o \quad (11)$$

From the orthogonality of the cosine functions, the Dirac delta function can be written (3):

$$\delta(f-f_o) = 4 \int_0^\infty \cos [2\pi(f-f_o)\tau] d\tau \quad (12)$$

where

$$\delta(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ \infty & \text{for } x = 0 \end{cases}$$

and

$$\int_{-\infty}^{\infty} \delta(x) dx = 1.$$

From equation (12), equation (11) can be written:

$$B_c(\sigma_c) = \int_0^{\infty} B_o(\sigma_o) \delta\left(\frac{\sigma_o}{n(\text{HeNe})} - \sigma_c\right) d\sigma_o. \quad (13)$$

Since only the alteration of the wavenumber scale is of interest, inspection of equation (13) shows that the delta function is zero except at,

$$\sigma_c = \frac{\sigma_o}{n(\text{HeNe})} \quad (14)$$

and since the observed wavenumbers are in air,  $\sigma_o$  can be written,

$$\sigma_o = n(\sigma_{\text{Vac}}) \cdot \sigma_{\text{Vac}} \quad (15)$$

where  $n(\sigma_{\text{Vac}})$  is the index of refraction of air at the vacuum wavenumber of the spectrum. From equations (14) and (15), the calculated wavenumbers,  $\sigma_c$ , can be related to the vacuum wavenumber of the observed spectrum by,

$$\sigma_c = \frac{n(\sigma_{\text{Vac}})}{n(\text{HeNe})} \cdot \sigma_{\text{Vac}} \quad (16)$$

The ratio of the indices of refraction of air in equation (16) is less than one for  $\sigma_{\text{Vac}}$  lying in the IR, so the calculated wavenumbers are less than the true (vacuum) wavenumbers. Consider the error,  $\Delta\sigma$ , resulting from equation (16):

$$\Delta\sigma = \sigma_{\text{Vac}} - \sigma_c = \sigma_{\text{Vac}} \left(1 - \frac{n(\sigma_{\text{Vac}})}{n(\text{HeNe})}\right).$$

At room temperature (22°C) and standard pressure (760mm) the error in the calculated wavenumbers at 2000  $\text{cm}^{-1}$  is .008  $\text{cm}^{-1}$  and at 4000  $\text{cm}^{-1}$  the error is .015  $\text{cm}^{-1}$ . It is therefore necessary that this error be considered if high precision wavenumber determination is desired. It should be pointed out that the errors described by equations (1) and (16) lead to a lower wavenumber scale than the true scale, thus their effects are additive.

A number of other errors can effect the precision of the wavenumber

scale on the FTS system; however, the errors summarized by equations (1) and (16) are both significant and readily correctable. Problems such as sampling errors, laser instability, and mirror-velocity fluctuations can lead to errors in wavenumber calibration, but these are normally characteristics of a particular FTS system, and may not be easily corrected. While equation (16) can supply a correction to the calculated wavenumber scale by knowing the index of refraction of air, the solid angle in equation (1) can be difficult quantity to accurately measure. One approach to determining the solid angle term in equation (1) is to compare measured line positions with known values. Then, theoretically, the correction term for equation (1) is known for the remainder of the wave number scale. This was the scheme chosen to calibrate the FTS wavenumber scale resulting in a calibration program, FTCAL, which is described in appendix III-1. Using known line positions (up to 100), the solid angle term,  $\Omega/4\pi$ , in equation (1) is determined by the method of least-squares after altering the known line positions according to equation (16). The reason for altering the known line positions before performing the least-squares calculation is so the only error remaining is that due to equation (1). After the least-squares calculation is performed, corrected values for the measured line positions are computed as follows;

$$\sigma_1 = \frac{\sigma \text{ (measured)}}{1 - \Omega/4\pi}$$

$$\sigma \text{ (corrected)} = \sigma_1 \cdot \frac{n(\text{HeNe})}{n(\sigma_1)} \quad (17)$$

The corrected values are compared with the (unaltered) known positions to determine the errors between the two sets. If the user has specified an inclusion/rejection criterion (the parameter PR in the program), the errors are compared with the value of PR to determine if a line should be excluded from the least-squares calculation.

If the largest error exceeds PR, the measured line position which yielded that error is excluded from the set of measured values, and the least-squares calculation is repeated. This process is repeated until only the lines yielding an error less than PR are included in the least-squares calculation of  $\Omega/4\pi$ . If PR is set equal to zero, all lines are included. After a value for  $\Omega/4\pi$  is found, unknown lines are read-in and corrected according to equations (17). The index of refraction of air is calculated using Edlen's formula and corrected for non-standard temperature and pressure using ideal gas law corrections [2]. The user of FTCAL must specify the temperature (deg. C) and barometric pressure (mm of Hg) at which the standard lines were measured and the unknown measurements made. It should be pointed out that if the temperature differs by less than  $\pm 5^\circ\text{C}$  and the pressure differs by less than  $\pm 20$  torr between the calibration measurement and the unknown measurement, the error resulting from assuming both were taken under the same conditions is less than  $.001\text{ cm}^{-1}$  over the wavenumber range  $400\text{ cm}^{-1}$  to  $4000\text{ cm}^{-1}$ . For a detailed description of FTCAL, the reader is referred to Appendix I.

Another area that needed investigating before making precision line position measurements involved the best methods for determining the line center with the FTS system. Two basic options are available to the FTS user. Firstly, the user may use the intensified cursor to directly read-out the line positions from the c.r.t. display and secondly, the user may read the line position values from a hard-copy plot of the data. The former method is very convenient, but suffers from poor consistency. The latter method is cumbersome and time consuming but yields good measurement consistency. Using the carbon monoxide fundamental as a known set of lines and the overtone as an unknown set (both are known to better than  $.0002\text{ cm}^{-1}$ ) evaluation of the FTS system and the FTCAL program was begun. From these measurements, a

number of guidelines developed. These are summarized below:

1. Dispersive elements (such as lenses) in the collimating optics lead to non-linearities in equation (1) and invalidate that correction if the unknown and known lines differ greatly in wavenumber.
2. Use of the intensified cursor to determine line positions can at best yield a precision of  $\pm 0.005 \text{ cm}^{-1}$ .
3. Use of the plotting routine with the FIT parameter set to YS can lead to a precision of better than  $\pm 0.002 \text{ cm}^{-1}$ . Use of the FIT routine is imperative for good interpolation between data points.
4. Line centers should be determined by using paper with a grid or overlaying plots on a grid. Plots should always be made of absorbance files unless absorbance values are small ( $<0.1$ ). Plots should be made using a scale factor of  $0.1 \text{ cm}^{-1}$  per inch or less.

It is felt that a precision of better than  $\pm 0.002 \text{ cm}^{-1}$  is obtainable over the wavenumber range  $400 \text{ cm}^{-1}$  to  $4000 \text{ cm}^{-1}$  and perhaps  $\pm 0.001 \text{ cm}^{-1}$  in the wavenumber range below  $2000 \text{ cm}^{-1}$ .



SECTION II  
ROTATIONAL AND VIBRATIONAL POPULATION  
DISTRIBUTION IN CARBON MONOXIDE

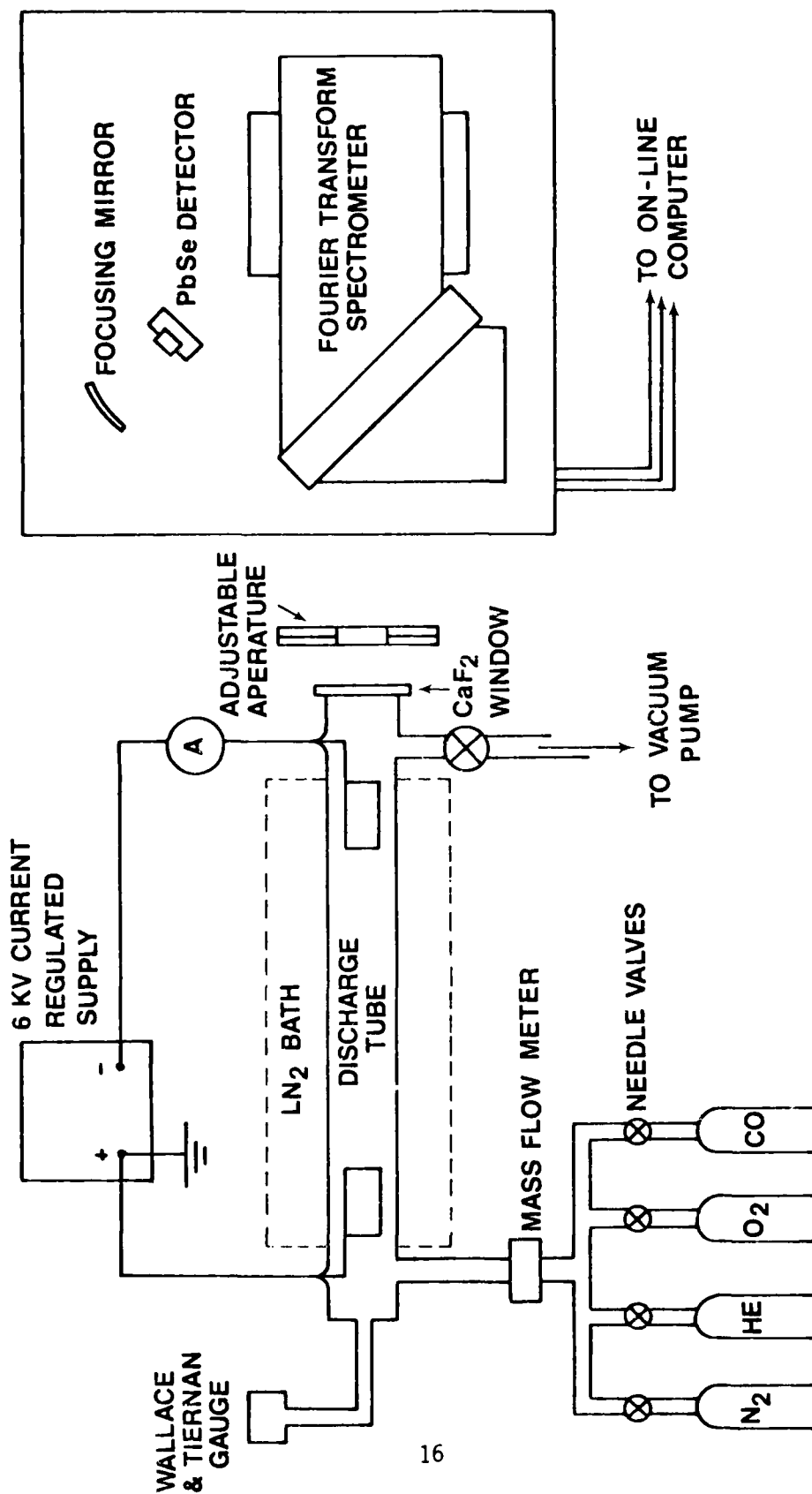
Determination of the rotational temperature and vibrational populations of carbon monoxide in a low pressure gas discharge has been accomplished. A computer code has been developed which allows the user to input low resolution emission data from either the fundamental, first, or second overtone of carbon monoxide and outputs to the user the rotational temperature and the fraction of molecules in each vibrational level. This investigation resulted in a paper being presented at a Mini Symposium on Aerospace Systems Technology - Present and Future, sponsored by the American Institute of Aeronautics and Astronautics.

Figure 4 shows the experimental setup used for making the measurements. Radiation leaving the discharge tube passed through the adjustable aperture, through the fourier transform spectrometer (FTS), and was then focused on the PbSe detector. The discharge tube was a cylinder roughly 2.5 cm. in. diameter and 50 cm. in length. The entire optical path was purged with dry air which was also free of carbon dioxide. Both water vapor and carbon dioxide parasitically absorb the infrared radiation from the discharge. The spectral regions in which these molecules absorb is illustrated in Figure 3, and partially overlaps the emission from CO.

When absorption due to  $\text{CO}_2$  and  $\text{H}_2\text{O}$  is not present, the spectrum of the emission from a  $\text{CO-N}_2\text{-He}$  discharge is illustrated in Figure 5. The band at  $2000\text{ cm}^{-1}$  is due to many overlapping fundamental transitions  $\Delta V=1$  while the band extending from  $2800$  to  $4400\text{ cm}^{-1}$  is due to many overlapping first overtone ( $\Delta V=2$ ) transitions. As shown schematically in Figure 6, each of the overtone transitions has a P and an R branch, but each successive

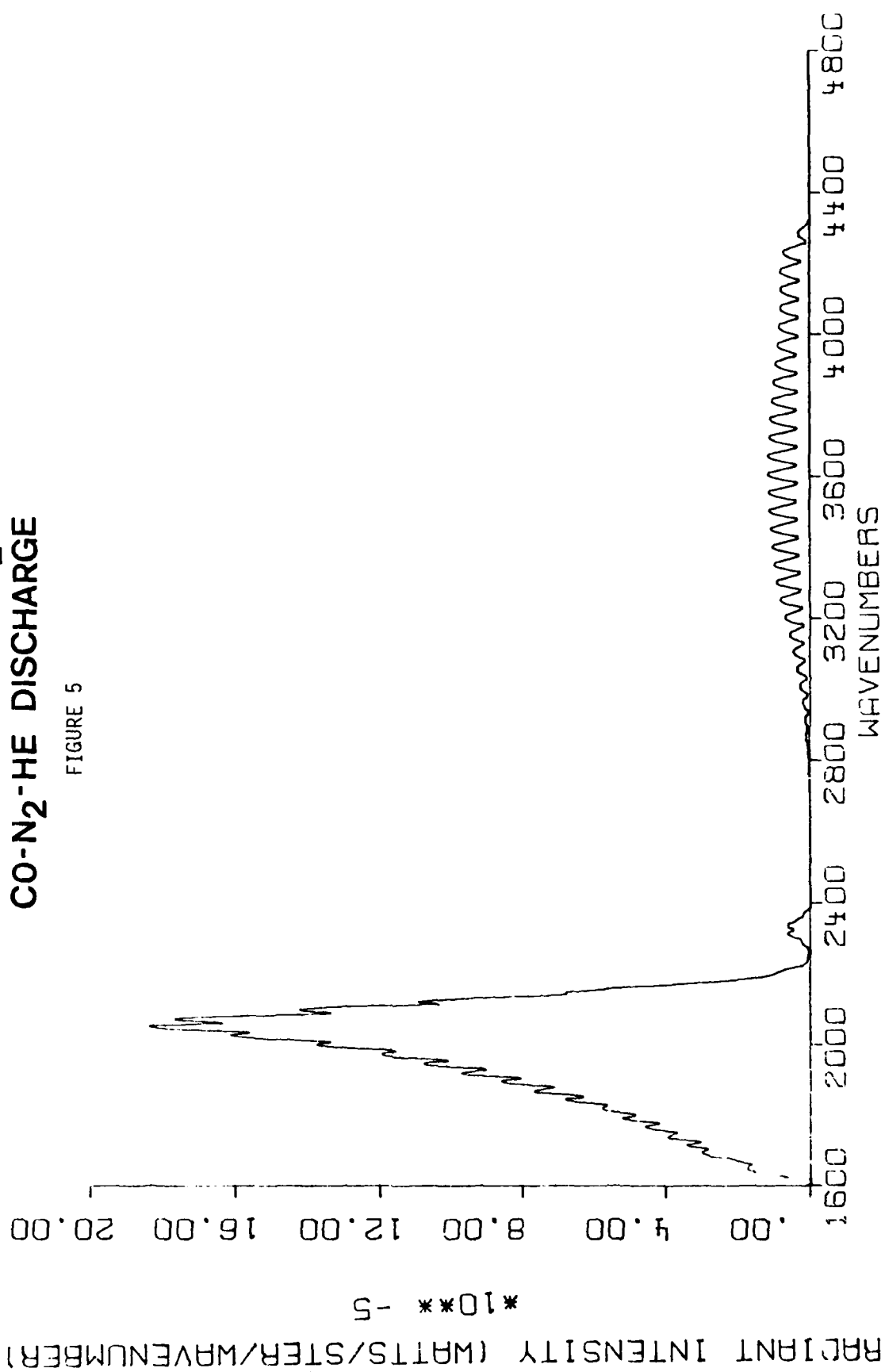
# SCHEMATIC OF THE EXPERIMENT

FIGURE 4

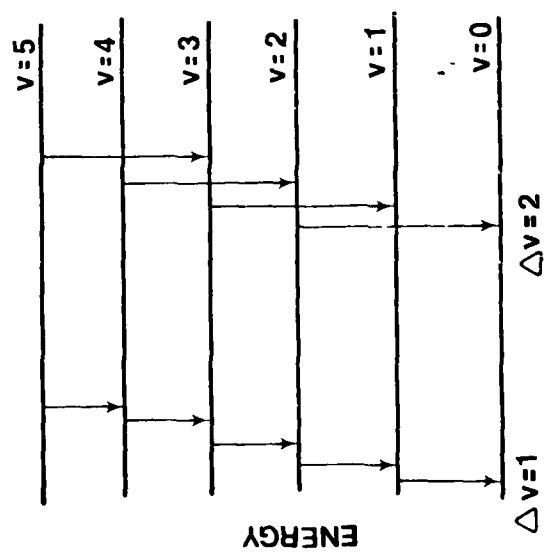


# LOW RESOLUTION INFRARED EMISSION SPECTRUM OF A LN<sub>2</sub>-COOLED CO-N<sub>2</sub>-HE DISCHARGE

FIGURE 5



FUNDAMENTAL ( $\Delta v=1$ )  
AND FIRST OVERTONE ( $\Delta v=2$ )  
VIBRATIONAL TRANSITIONS



OVERLAP OF THE VIBRATIONAL  
BANDS IN THE FIRST  
OVERTONE

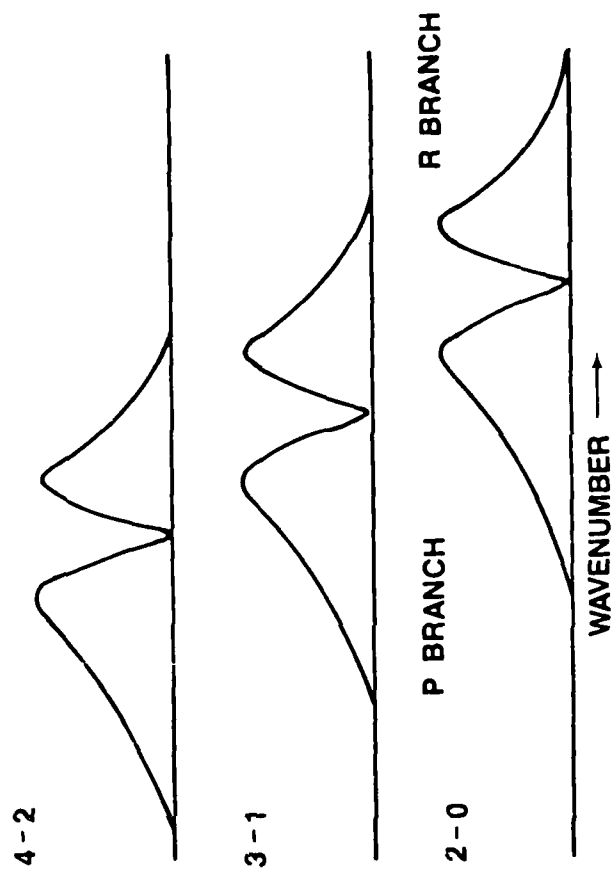


FIGURE 6

transition is shifted to lower wavelength because of vibrational anharmonicity. The observed spectrum is the overlap of many slightly shifted P and R branches. It should be noted in Figure 5 that the R-branch of the  $V = 2$  to  $V = 0$  transition is not overlapped by any other bands, hence the theoretical description of the intensity in this region is greatly simplified. Figure 7 is detailed plot of the CO first overtone emission showing the structure resulting from more than 30 vibrational levels contributing to the spectrum.

The approach taken to the problem of determining the rotational temperature and vibrational populations from data typified in Figure 7 was guided by three primary considerations. First, determine the rotational temperature and vibrational populations that yield a "best fit" between a measured and a theoretical first overtone spectrum. Second, the computation should be efficient and free from "trial and error" fitting procedures. Third, because of the non-equilibrium nature of the problem, no assumption about the behavior of the vibrational populations can be made. In addition, two assumptions made in the approach were that the distribution of molecules among rotational lines could be treated as delta functions.

The method of solution developed from this approach is outlined below.

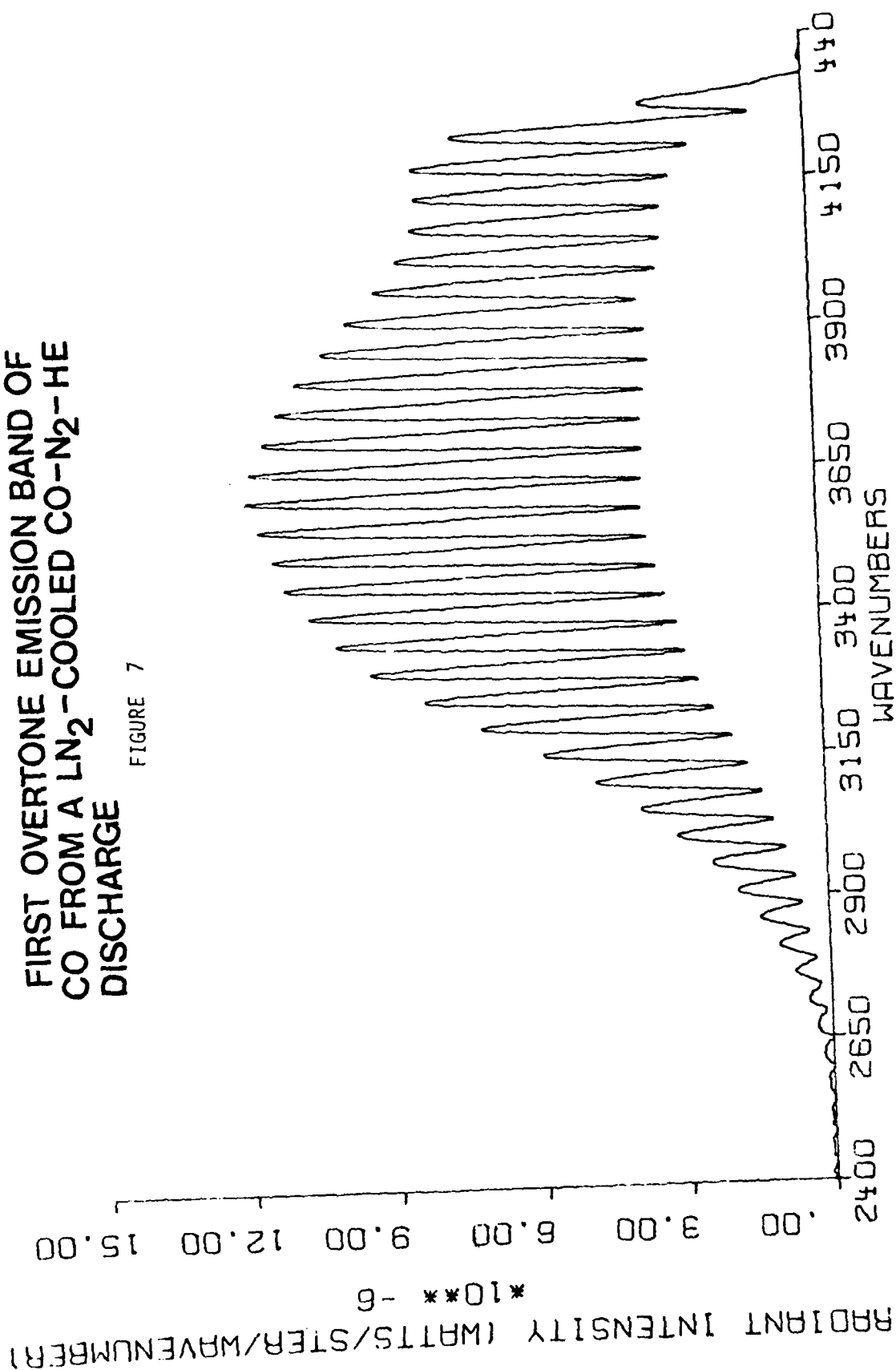
I. Correct the measured spectrum for the instrument response function.

The instrument response function (IRF) is found by dividing a measured black body spectrum by the theoretical black body spectrum. Raw spectral data is subsequently corrected by dividing by the IRF. This procedure removes effects due to beamsplitter variations, detector sensitivity, amplifier gain, etc. The spectra shown were corrected in this manner.

II. Calculate the rotational temperature from the R-branch of the 2-0 transition. Because the 2-0 R-branch is not overlapped

FIRST OVERTONE EMISSION BAND OF  
CO FROM A LN<sub>2</sub>-COOLED CO-N<sub>2</sub>-HE  
DISCHARGE

FIGURE 7



by other bands, the shape only depends on  $T_{ROT}$  and the  $V = 2$  number density. These parameters are determined by performing a two parameter, non-linear least squares fit between the measured and theoretical 2-0 R-branch.

- III. Calculate the vibrational populations using data from full overtone spectrum. Using  $T_{ROT}$  from II, a theoretical overtone spectrum is generated which is a function of the number densities in each vibrational level. A multiple linear regression analysis is then used to determine the set of vibrational populations that yield a best fit.
- IV. Compare the resulting theoretical spectrum with the measured spectrum. Step I is performed on the FTS data system while the remaining steps are performed on a CDC 6600 by the computer code CODIAG. A listing of this code is Appendix II. Data points are taken from the FTS data system and manually punched on cards for the 6600.

A map of the structure of CODIAG is shown in Figure 8. The first step in the analysis is to determine the rotational temperature from the spectral data of the R-branch of the 2-0 transition. The intensity of the CO emission in this region can be written as,

$$I(\sigma) = N_2 f(\sigma; T_R) \quad (18)$$

where  $I(\sigma)$  is the intensity at wavenumber  $\sigma$ ,  $N_2$  is the number of CO molecules in the  $v=2$  level, and  $f(\sigma; T_R)$  is a function which is non-linear in the rotational temperature,  $T_R$ . The behavior of the function  $f(\sigma; T_R)$  is the result of the intensity distribution among the rotational lines of the 2-0 R-branch folded with the spectrometer instrument function. The unknown parameters  $N_2$  and  $T_R$  in equation (18) are determined from a set of measured

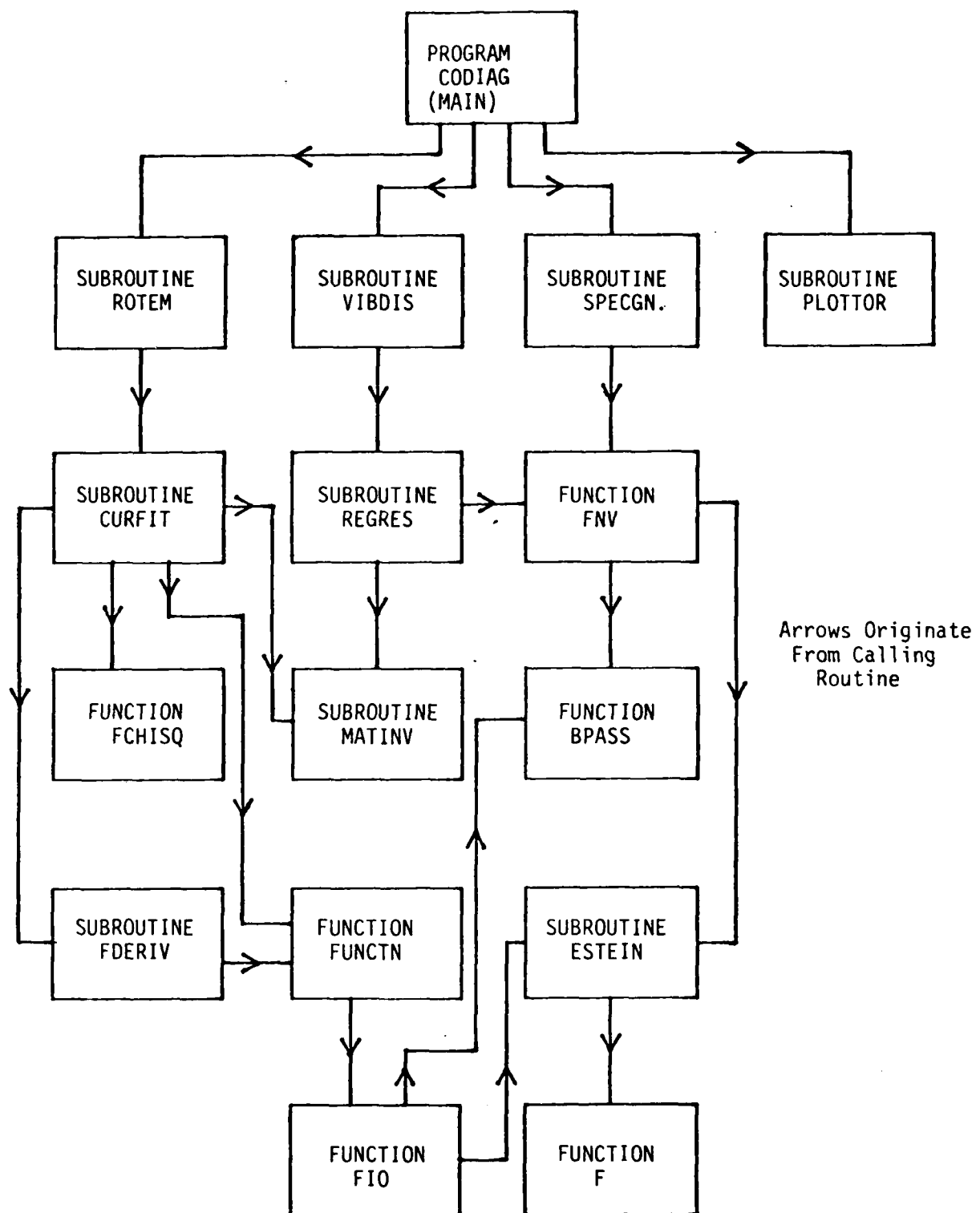


FIGURE 8 PROGRAM STRUCTURE OF CODIAG



intensities  $\{I(\sigma_i)\}$  using the non-linear least-squares fitting procedure developed by Marquardt [4] and described in Bevington [5]. The technique is iterative and requires initial guesses for  $N_j$  and  $T_R$ . This procedure is applied through the CODIAG SUBROUTINE ROTEM. Initial guesses and data input is through ROTEM while the actual least-squares algorithm is contained in SUBROUTINE CURFIT which is modified version of a program appearing in Bevington [5]. The right side of equation (18) is calculated in FUNCTION FIO which is called by CURFIT through the intermediary FUNCTION.

The intensity at any point in the calculated spectrum can be written

$$I(\sigma_i) = \sum_{j=2}^n N_j f_j(\sigma_i; T_R) \quad (19)$$

where  $N_j$  is the number of molecules in the  $j^{\text{th}}$  vibrational level and  $f_j(\sigma_i; T_R)$  includes the behavior of the rotational intensity distribution folded with the spectrometer instrument function. Since  $T_R$  has already been found, write  $f_j(\sigma_i; T_R)$  as  $f_j(\sigma_i) \equiv f_{ji}$ . Then equation (19) becomes

$$I(\sigma_i) = I_i = \sum_j N_j f_{ji} \quad (20)$$

Since the measured intensities might contain a zero offset, the function used to describe the measured spectrum is written

$$I_i = \alpha_0 + \sum_j N_j f_{ji} \quad (21)$$

It is desired then to find the set  $\{N_j\}$  from a measured set of intensities  $\{Y_i\}$ . The method chosen for this is to minimize the function  $\chi^2$  by adjusting the set  $\{N_j\}$ .  $\chi^2$  is given by

$$\chi^2 = \sum_i \frac{1}{\Delta_i^2} (Y_i - I_i)^2 \quad (22)$$

where  $\Delta_i$  is the standard deviation of the  $i^{\text{th}}$  measured intensity. At the minimum of  $\chi^2$ , the partial derivatives of  $\chi^2$  with respect to  $\alpha_0$  and each parameter  $N_j$  are zero or

$$\frac{\partial \chi^2}{\partial \alpha_0} = \frac{\partial \chi^2}{\partial N_2} = \dots = \frac{\partial \chi^2}{\partial N_n} = 0 \quad (23)$$

Substitute equation (21) into equation (22) and apply condition (23) yields a set of linear equations which can be solved for  $\alpha_0$  and the set  $\{N_j\}$ . The reader is referred to Bevington [5] for a detailed description of the solution. The application of this scheme to determine the set  $\{N_j\}$  is through SUBROUTINE VIBDIS (See Figure 8). The actual multiple linear regression is performed in SUBROUTINE REGRES which is a modified version of a program appearing in Bevington [5]. The functions  $f_{ji}$  in equation (21) are calculated in FUNCTION FNV. In addition to handling the data I.O. from the vibrational population determination, VIBDIS also calculates values for  $N_0$  and  $N_1$  from an assumed Treanor distribution [6] over the lower vibrational level. The Treanor distribution can be written as

$$N_v = N_0 \cdot \exp (v\theta - E_v/kT) \quad (24)$$

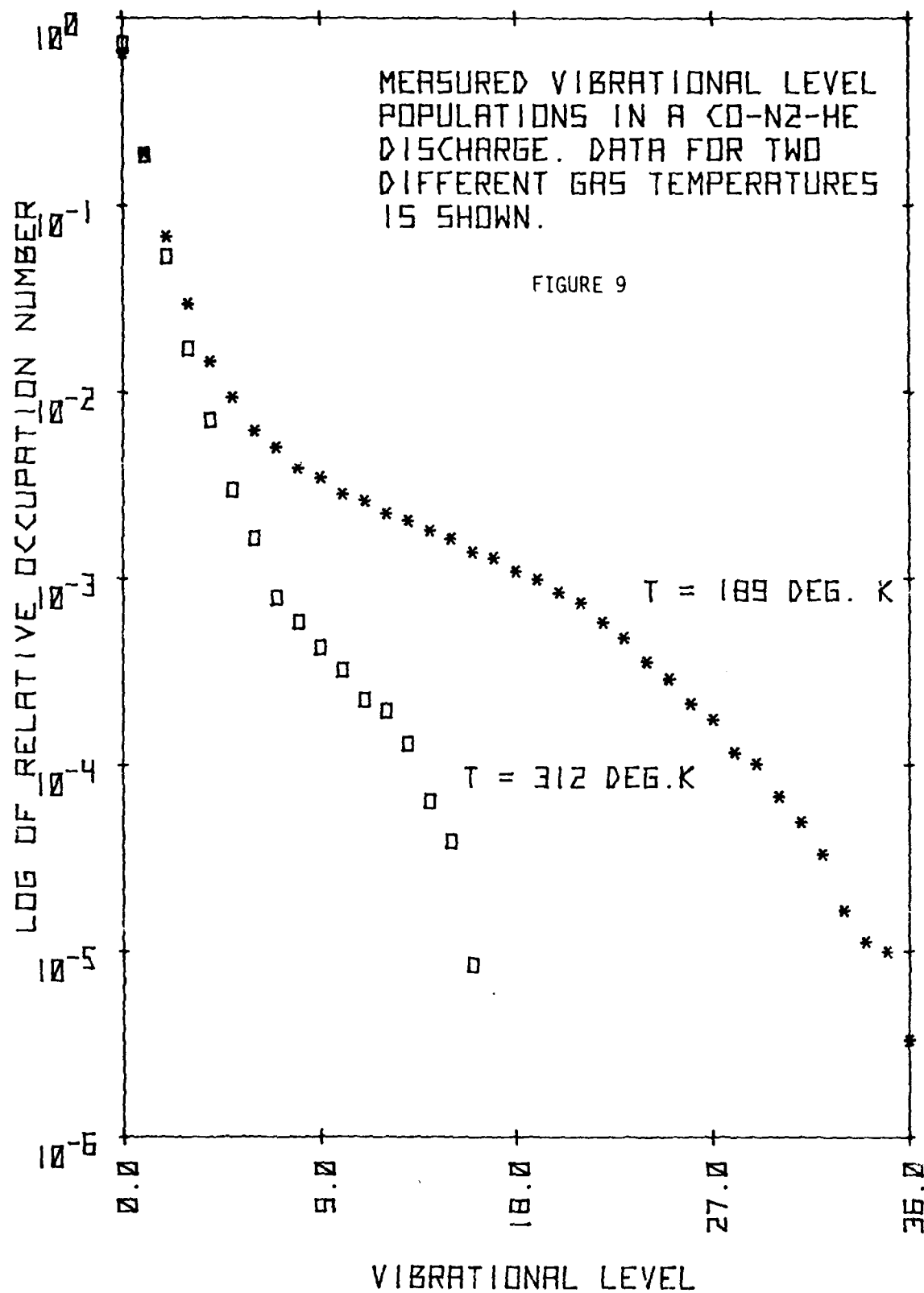
where  $E_v$  is the energy of the  $v^{\text{th}}$  vibrational level compared to the  $v=0$  energy,  $\theta$  is a constant at a fixed gas temperature,  $k$  is the Boltzmann constant, and  $T$  is the kinetic (and rotational) temperature of the gas. The value of  $\theta$  can be determined from equation (24) with the previously determined values of  $N_2$  and  $N_3$  and is given by

$$\theta = \ln \left( \frac{N_3}{N_2} \right) + (E_3 - E_2) / kT \quad (25)$$

Using equation (25) and equation (24), along with the calculated values for  $N_2$  and  $N_3$ , the Treanor values for  $N_0$  and  $N_1$  can be found.

As an initial test of CODIAG, data points were taken from a synthetic spectrum generated from a known  $T_R$  and a known set  $\{N_j\}$  and input into CODIAG. This test would indicate if the program could determine  $T_R$  and the set  $\{N_j\}$  from a limited number of data points. The results for a 30 level set  $\{N_j\}$  were excellent. A more difficult test was to determine the desired parameters from a measured spectrum. Data was obtained from a liquid nitrogen cooled CO-N<sub>2</sub>-He discharge with a 1:2:10 mixture ratio and operating at a pressure of about 1 torr. The discharge length was about 50 cm and the current and voltage were 15 mA at 4.9 Kv. In addition, about .15% of the total pressure was oxygen. The measured overtone spectrum is shown in Figure as obtained with a Fourier Transform Spectrometer with a resolution of about  $10\text{cm}^{-1}$ . Calibration of the system was achieved by comparing a theoretical 700°K black body function with a measured spectrum from a standard source. Eighteen data points were taken from the R-branch of the 2-0 transition for the determination of  $T_R$  and an additional seventy four data points were taken throughout the spectrum for determination of the vibrational populations. The data points chosen were primarily the "peaks" and "valleys" of the vibrational structure in the spectrum. The rotational temperature was found to be 207°K with an estimated uncertainty of  $\pm 10^\circ\text{K}$ . The calculated vibrational population distribution is illustrated in Figure 9, which is a plot of the log of the relative occupation number versus vibrational level. The relative occupation number is given by  $N_j/\sum N_j$ .

Also shown in Figure 9 is the population distribution from a room temperature discharge shown in Figure 10. The stars correspond to the data in Figure 7 and the rectangles correspond to the data in



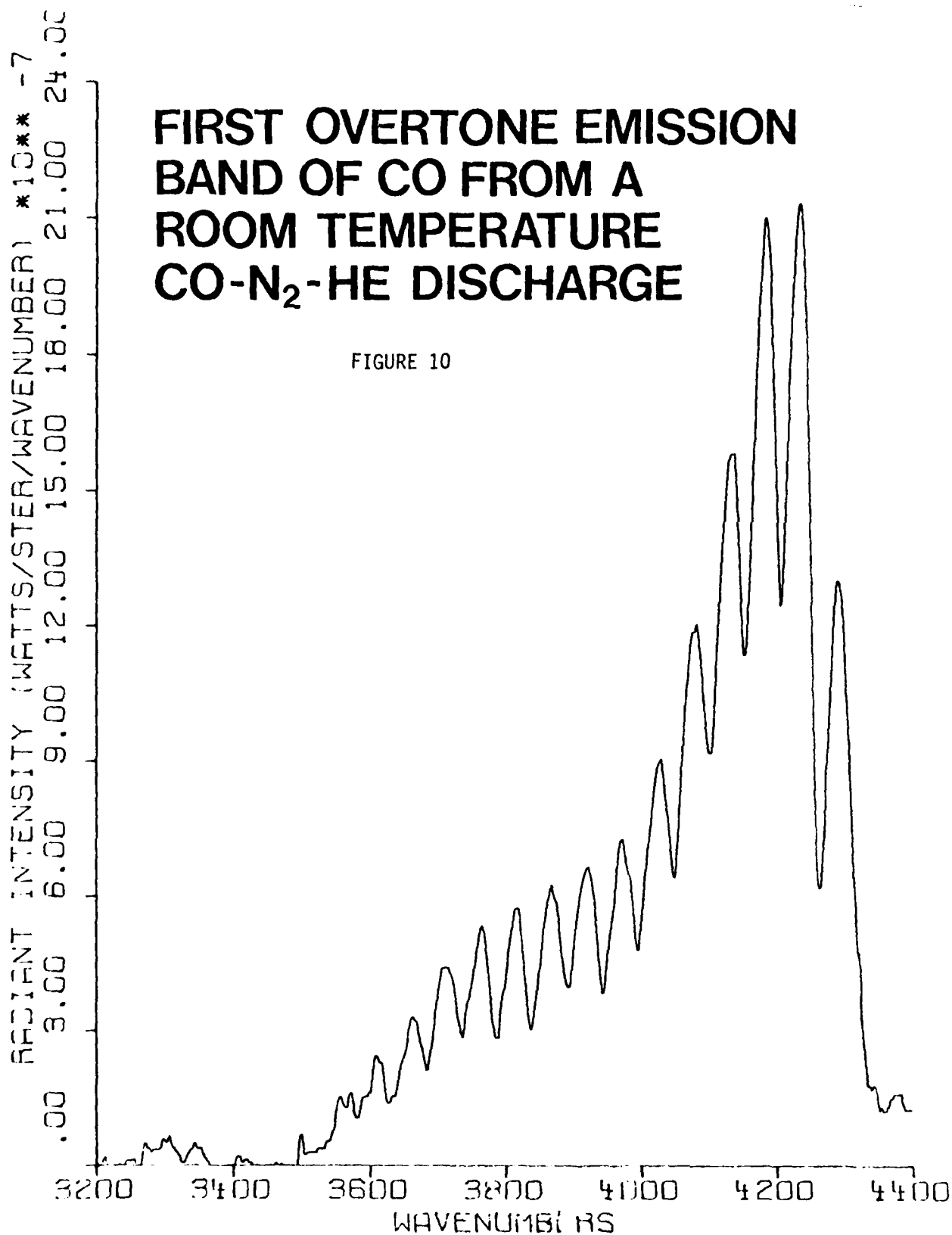
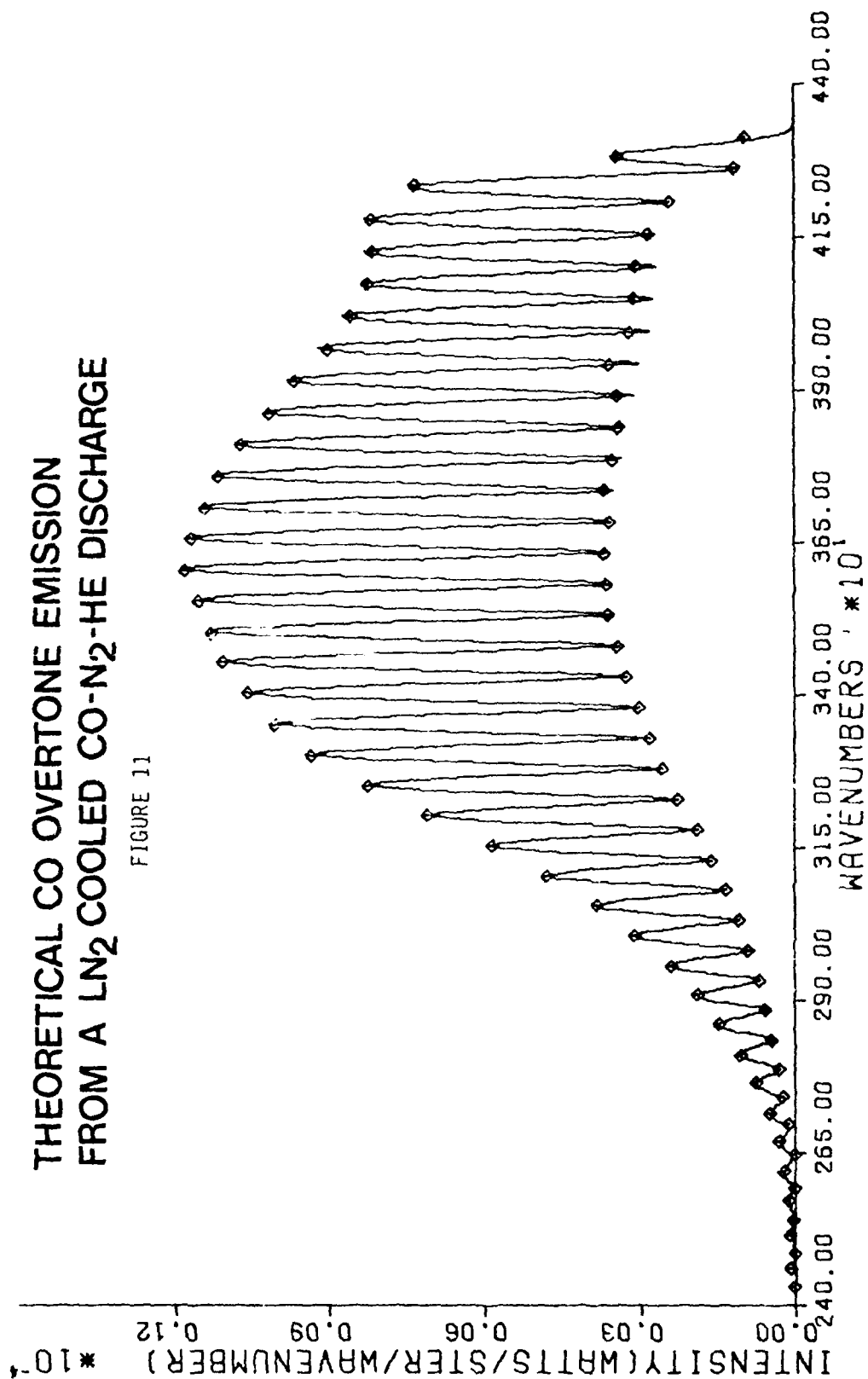


Figure 10. The theoretical spectra calculated from these vibrational populations and rotational temperature are shown in Figure 11 and Figure 12. In these figures, the small diamonds indicate the data points used in the analysis. Figure 11 and Figure 12 can be compared with Figure 7 and Figure 10 as an indication of the confidence in the results shown in Figure 9.

From the results shown here, some conclusions can be drawn as to the limitation of the diagnostics along with some guidelines for determining its sensitivity. With a signal-to-noise ratio (S/N) on the order of 100, vibrational population data has been calculated over 5 orders of magnitude. With a S/N on the order of 65 in the 2-0 R-branch, the estimated standard deviation in  $T_{ROT}$  is less than 5% of  $T_{ROT}$ . It appears that a good estimate of the relationship between S/N in the R-branch and the standard deviation in  $T_{ROT}$  is given by  $(\Delta T/T) \cdot (S/N) \approx 1.3$ . The chief sources of error in the calculation of the vibrational populations are probably systematic. Errors in correcting for system sensitivity and errors in calculating the CO transition probabilities are probably large compared to the fluctuations in the vibrational populations due to a S/N greater than 20. Measurement times can be shortened, down to the time required for a single scan of the FTS, with a corresponding decrease in S/N. Single scan times can be less than 0.1 sec. with an effective noise equivalent power of  $\approx 7 \times 10^{-10}$  watt/cm<sup>-1</sup> at 4000 cm<sup>-1</sup>. This effective NEP includes detector noise plus electronic noise and is adjusted for the system response function. Hence, if the radiant intensity of a source is known and the solid angle subtended at the FTS detector, this effective NEP can be used to give an estimate of the single scan S/N that can be expected. Inherent in the FTS technique is the need for sources to subtend a small solid angle

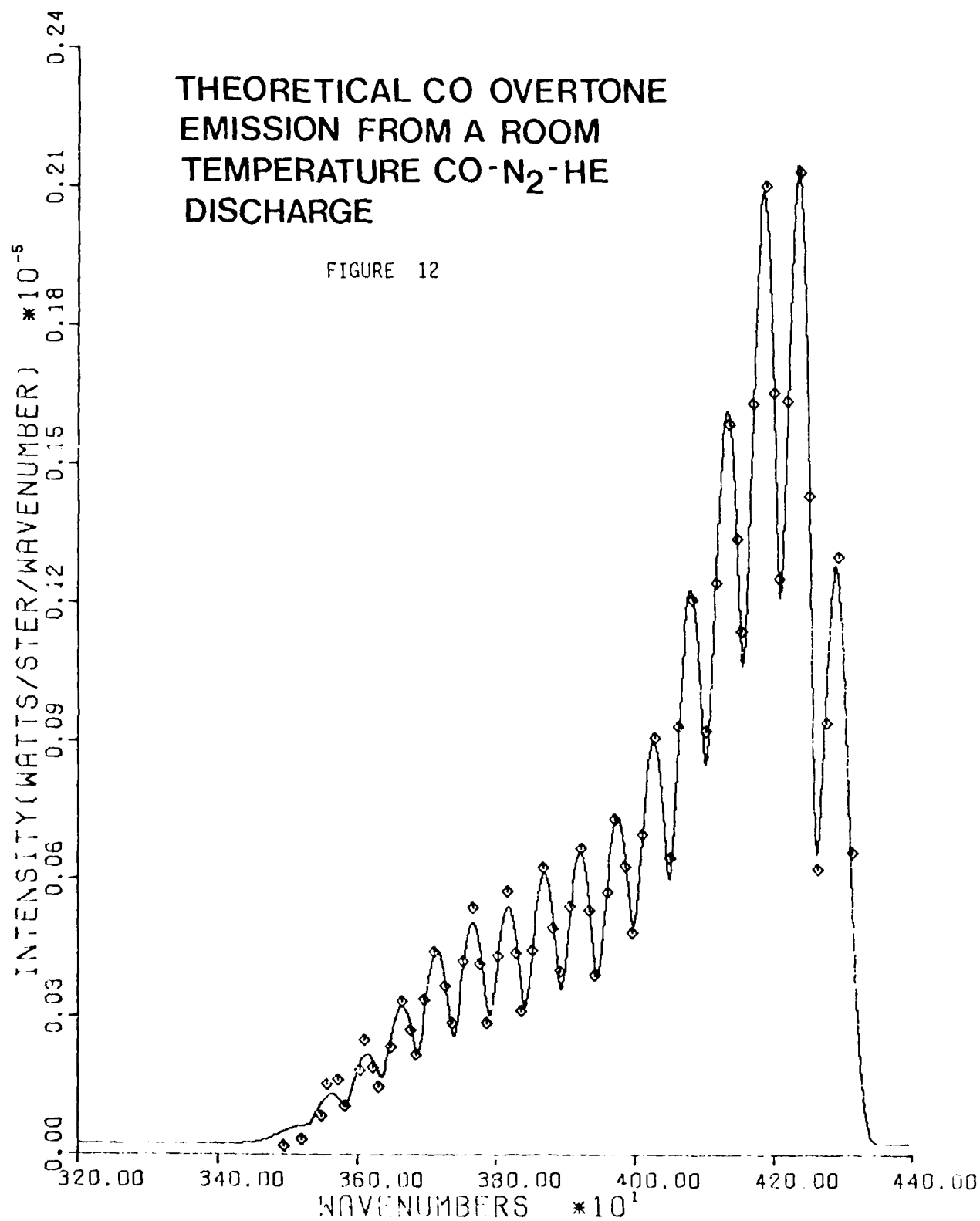
# THEORETICAL CO OVERTONE EMISSION FROM A LN<sub>2</sub> COOLED CO-N<sub>2</sub>-HE DISCHARGE

FIGURE 11



THEORETICAL CO OVERTONE  
EMISSION FROM A ROOM  
TEMPERATURE CO-N<sub>2</sub>-HE  
DISCHARGE

FIGURE 12





at the detector; however, for low resolution this requirement is not as stringent as needed for high resolution. For the resolution needed in this analysis, the source may subtend a solid angle as large as  $6 \times 10^{-7}$  ster. without degrading the technique. Lastly, it should be pointed out that absorption by water vapor in the optical path would completely prohibit obtaining vibrational population data; however,  $T_{\text{ROT}}$  is still measureable because the 2-0 R-branch lies outside the water vapor band.

### SECTION III

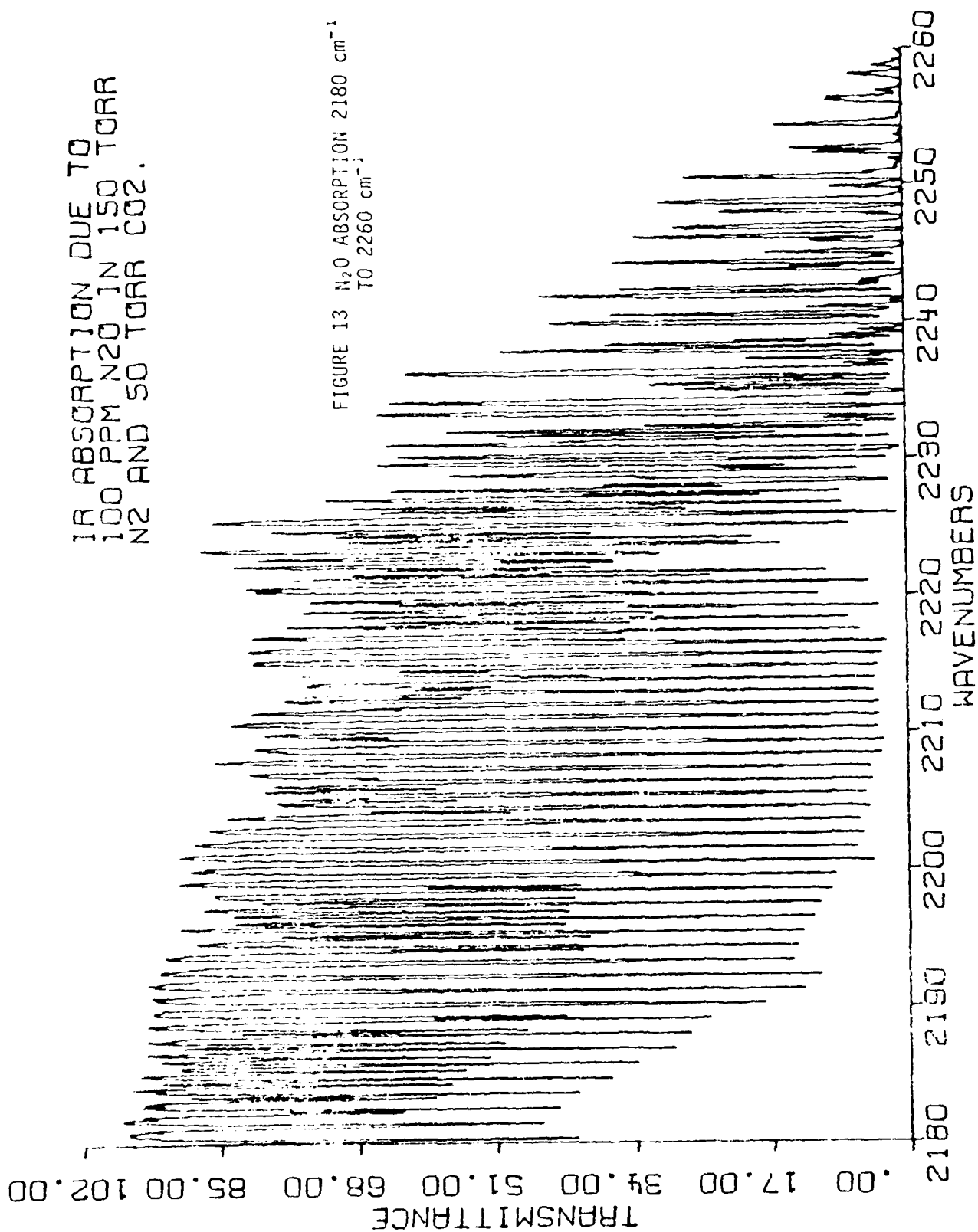
#### ABSORPTION BY DISCHARGE IMPURITIES

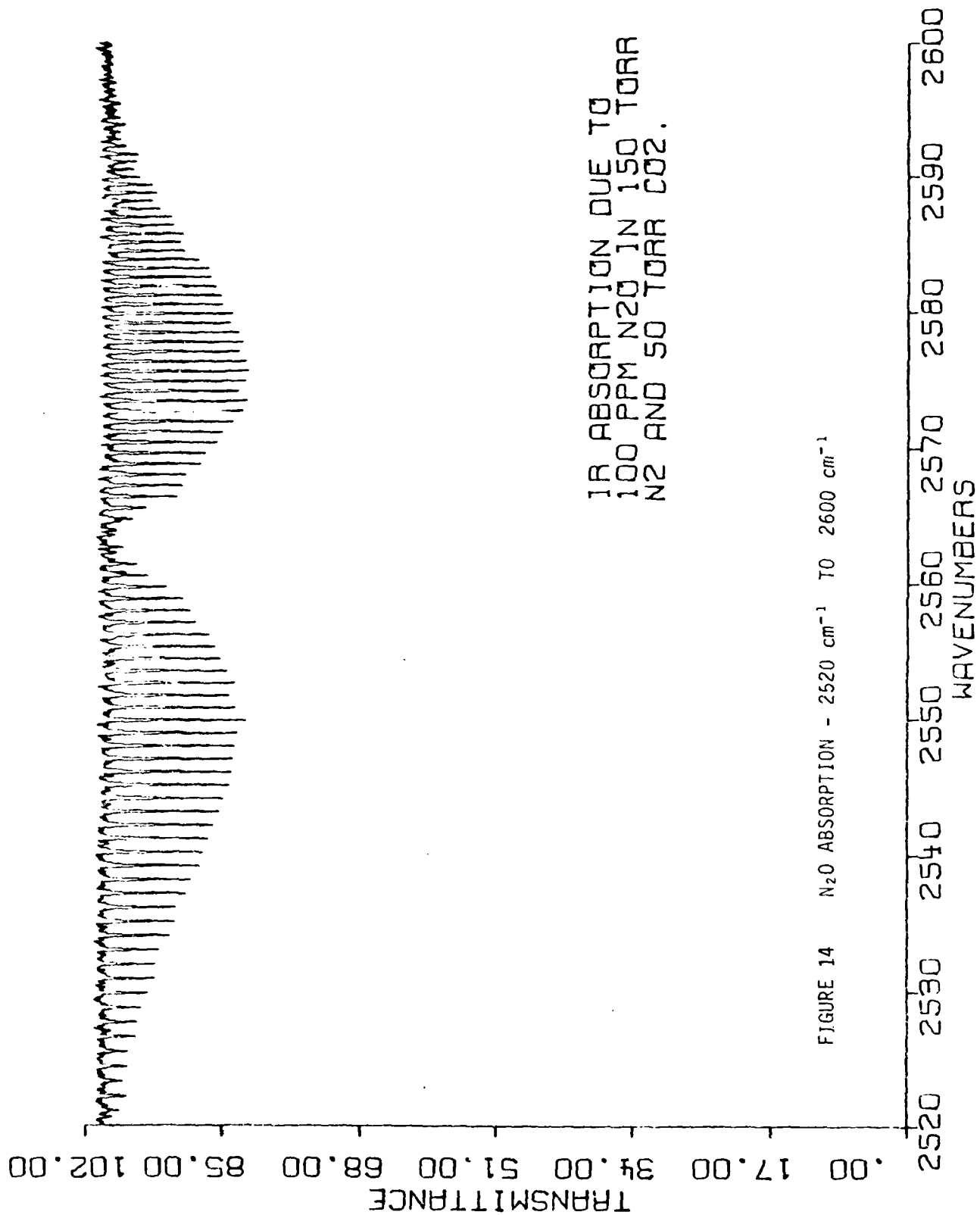
A number of gas mixes which model the gas found in the electron beam closed cycle discharge were studied in an effort to determine detection sensitivities for a number of minor species.

The first trace species studied were  $N_2O$ ,  $NO$ , and  $NO_2$ . These were chosen for their strong absorption bands in the PbSe region and their suspected presence in  $CO_2$  laser discharges. Gas mixes of 3 parts  $N_2$ , 1 part  $CO_2$  and various concentrations of the nitrogen oxides were made up and their absorption spectra obtained. Total pressure in the White cell was kept at 200 torr. This was done for the following reasons. First, below one half atmosphere the line widths of the trace species are on the order of the best spectral resolution obtainable with the FTS System ( $.06\text{ cm}^{-1}$ ). Thus, below  $\approx 380$  torr, the observed line widths should be pressure independent and interference between neighboring lines will be at a minimum. Second, the ratio of the volumes of the available sample cylinders to the White cell volume is about 1:5, so with an EBCC pressure of 1 atm., the White cell pressure should be on the order of 150 torr. Running the gas mixes at 200 torr was a reasonably good approximation to the conditions under which samples were to be studied.

With the gas mix just discussed,  $N_2O$  shows two reasonably strong absorption bands that are free from interfering species. The bands originate from the  $00^0_1 \rightarrow 00^0_0$  and  $20^0_0 \rightarrow 00^0_0$  transitions and are centered at  $2223.8\text{ cm}^{-1}$  and  $2563.3\text{ cm}^{-1}$  respectively [7]. Figure 13 shows a portion of the P-branch of the  $00^0_1 \rightarrow 00^0_0$  band while Figure 14 shows both branches of the  $20^0_0 \rightarrow 00^0_0$  band. These spectra were obtained with 100 ppm  $N_2O$

IR ABSORPTION DUE TO  
100 PPM N<sub>2</sub>O IN 150 TORR  
N<sub>2</sub> AND 50 TORR CO<sub>2</sub>.





in the 3:1  $\text{N}_2:\text{CO}_2$  gas mix previously discussed. The P-branch of the  $00^01 \rightarrow 00^00$  transition lies at the edge of strong absorption by a number of  $\text{CO}_2$  bands; thus there is some interference with the lower J-value  $\text{N}_2\text{O}$  lines. The R-branch of the  $00^01 \rightarrow 00^00$  transition is completely obscured by the  $\text{CO}_2$  absorption. Figure 15 shows the same spectral region as Figure 13 only the  $\text{N}_2\text{O}$  is missing from the gas mix and the  $\text{CO}$  pressure is somewhat higher. It can be seen that above about  $2200 \text{ cm}^{-1}$  interference from  $\text{CO}_2$  prohibits the use of the  $\text{N}_2\text{O}$  lines for determining its presence. The  $20^00 \rightarrow 00^00$  band lies in an interference-free region, but lacks the strong absorption of the  $00^01 \rightarrow 00^00$  band. Table 1 is a summary of the results for the two  $\text{N}_2\text{O}$  bands along with expected band strengths for the two bands studied. Lines are chosen based on the criteria of being relatively interference-free and showing strong absorption. The effective absorption coefficient was calculated from the slope of the straight line found by a least squares fit of concentration dependence of absorption. Errors were calculated assuming a 1% error in the transmission measurements which was roughly the noise level of 2000 sec. run with the PbSe detector. The transmission through the gas is given by:

$$I = I_0 e^{-\alpha p} \quad (26)$$

where (in this case),  $\alpha$  is in units of  $\text{torr}^{-1}$  and hence  $p$  is the partial pressure in torr. The estimated detection limit for each band shown in Table 1 is found by assuming a value of  $I/I_0$  of .995 can be measured (with the new InSb detector), and finding the pressure that yields this value. The estimate is good at a total pressure of 200 torr and changes with total pressure. Below about one half atmosphere, the detection limit is expected

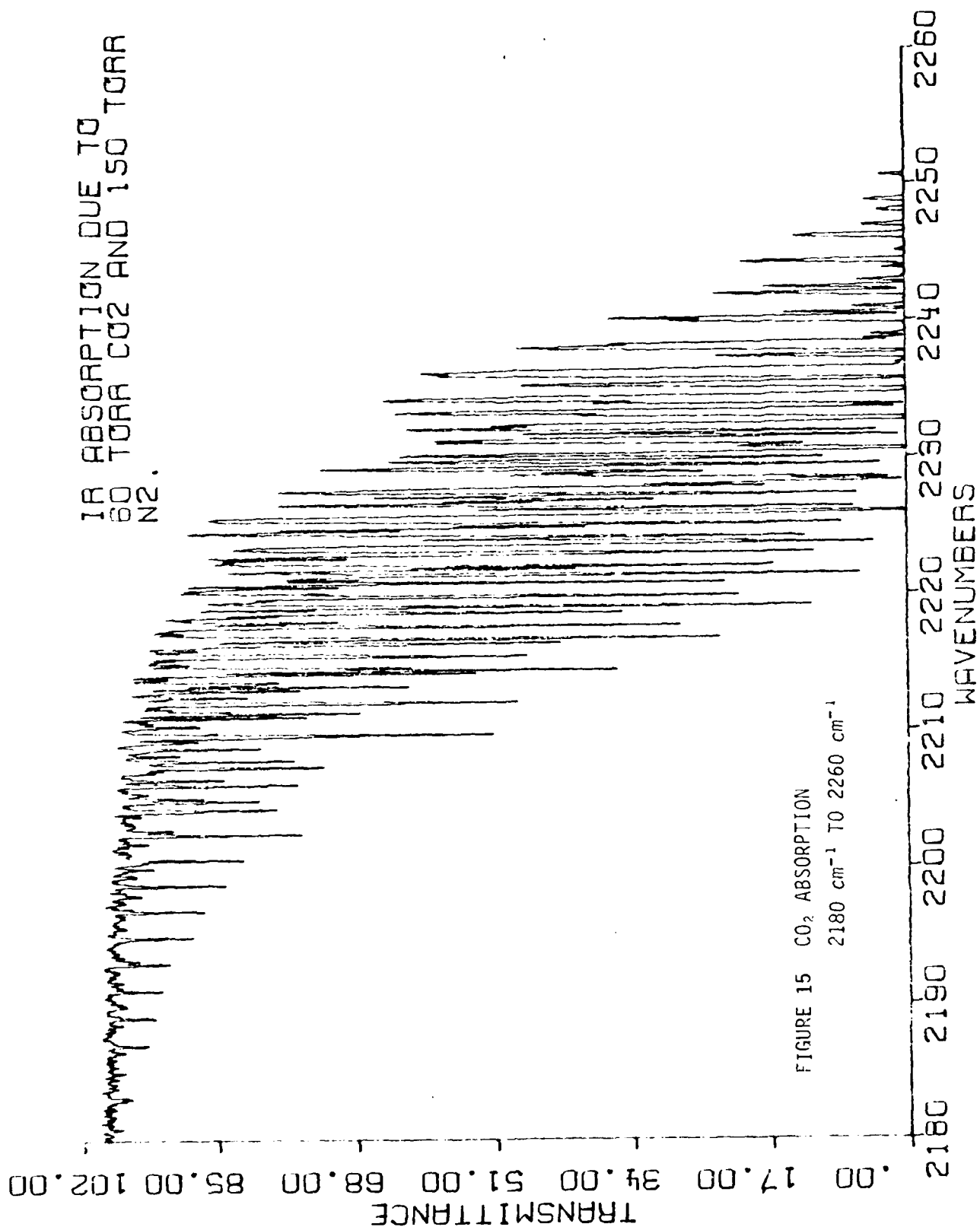


TABLE 1  
ABSORPTION DATA FOR NITROUS OXIDE

Band (Ref. 7)	Band Strength (Ref. 7) $\text{cm}^{-1}/\text{cm-atm}$	Line Identification (Ref. 8)	Line Position (Ref. 8)	Measured Effective Absorption Coefficient ( $\text{Torr}^{-1}$ )	Estimated Detection Limit (At 200 Torr Total Pressure)	Interfering Species
$00^0 1 \rightarrow 00^0 0$	$1536 \pm 67$	P(37)	2188.1898	$58.99 \pm 1.37$	$\approx .4 \text{ ppm}$	CO (Strongly Interfering) CO <sub>2</sub>
		P(36)	2189.2734	$63.97 \pm 1.50$		
		P(35)	2190.3502	$79.58 \pm 1.96$		
		P(34)	2191.4203	$102.7 \pm 2.8$		
		P(33)	2192.4837	$113.7 \pm 3.2$		
$20^0 0 \rightarrow 00^0 0$	$36.3 \pm 1.9$	P(17)	2548.1716	$9.47 \pm .85$	$\approx 2.5 \text{ ppm}$	None
		P(16)	2549.1178	$9.98 \pm .85$		
		P(15)	2550.0573	$10.04 \pm .86$		
		P(14)	2550.9901	$9.59 \pm .85$		
		P(13)	2551.9162	$9.17 \pm .84$		
		P(12)	2552.8355	$9.08 \pm .84$		
		R(12)	2573.6132	$10.17 \pm .86$	$\approx 2.5 \text{ ppm}$	None
		R(13)	2574.3556	$9.10 \pm .86$		
		R(14)	2575.0912	$9.88 \pm .86$		
		R(15)	2575.8199	$10.51 \pm .86$		
		R(16)	2576.5418	$9.75 \pm .86$		
		R(17)	2577.2569	$9.78 \pm .86$		

to increase linearly with decreasing total pressure while above one-half atmosphere the detection limit should be roughly constant due to pressure broadening. For example, for the  $00^0 1 \rightarrow 00^0 0$  band the minimum detectable amount of  $N_2O$  at 100 torr total pressure would be roughly twice the value given while at atmospheric pressure the value would be somewhat less than the given value.

The fundamental band of nitric oxide, centered near  $1876\text{ cm}^{-1}$ , lies in a region of strong water vapor absorption. While the P-branch lies in the stronger part of the  $H_2O$  band, the R-branch is overlapped by the  $11^1 0(2) \rightarrow 00^0 0$  band of  $CO_2$  [7] (the number in parenthesis locates the level in the Fermi resonating group). Due to the high number densities of  $CO_2$  in this experiment, it was decided to use lines of the P-branch that were not too strongly overlapped by  $H_2O$  lines. Table 2 gives the results of the measurements on NO and Figure 16 shows a typical absorption spectrum of the selected NO lines. The numbers arrived at in Table 2 were found in the same manner as in the  $N_2O$  data with one exception. The estimated detection limit was based on being able to measure a transmittance of 99% as opposed to 99.5% for the  $N_2O$  data. This was done because of the poorer signal-to-noise level in the  $1800\text{ cm}^{-1}$  region of the InSb detector.

The strongest  $NO_2$  band in the IR is the  $\nu_3$  band centered at  $1362.03\text{ cm}^{-1}$  [Ref. 9]. An average of the bandstrength measurements for this band yield a value [9] of  $848\text{ cm}^{-1}/\text{cm-atm.}$  which is somewhat larger than one half the  $N_2O$   $\nu_3$  bandstrength. The difficulty in using this band for detecting  $NO_2$  is that it lies in the middle of a very strong water vapor band which blocks most of the  $NO_2$  signal. Figure 17 shows the water vapor absorption in this region as a result of the spectrometer operating in laboratory air. The



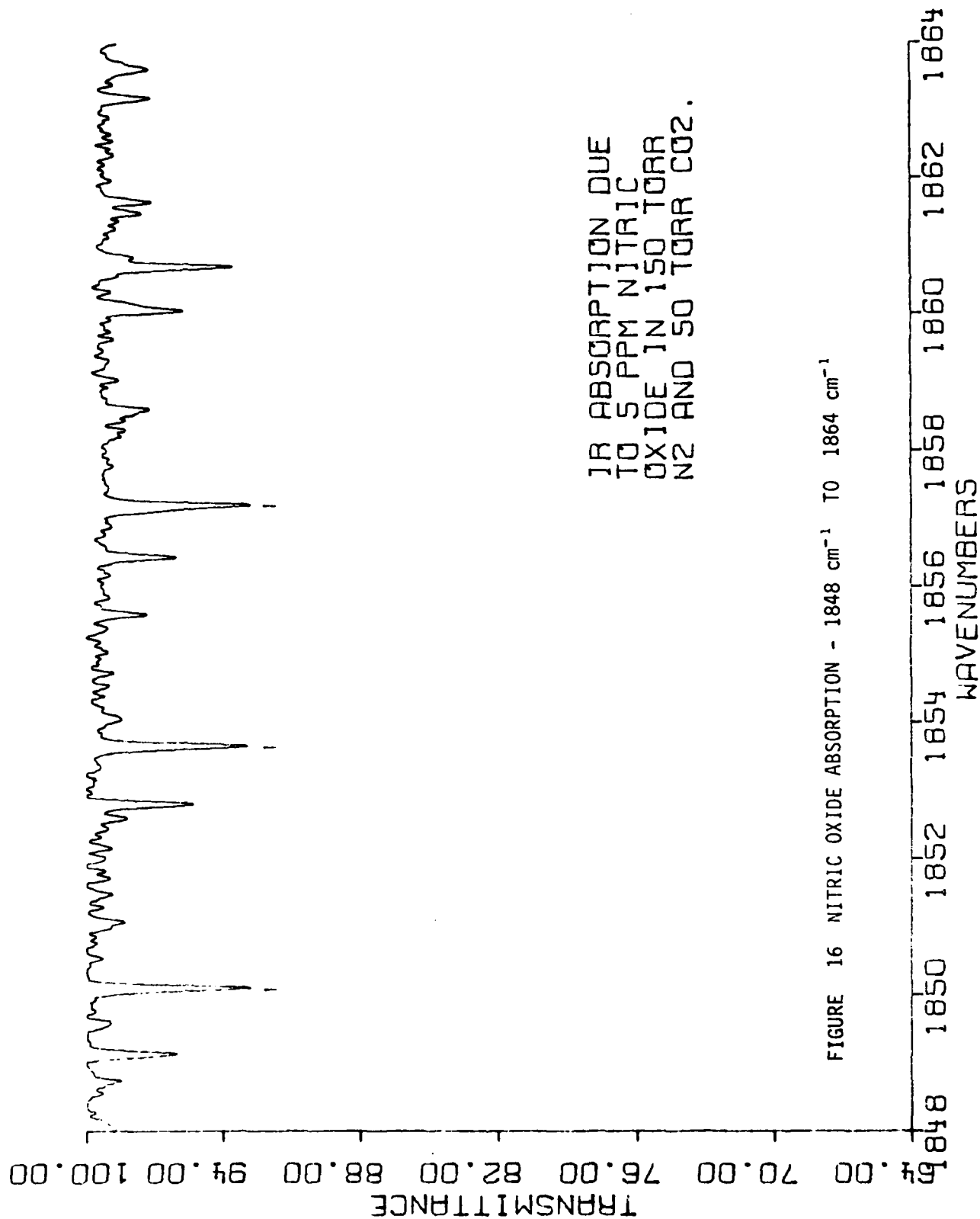
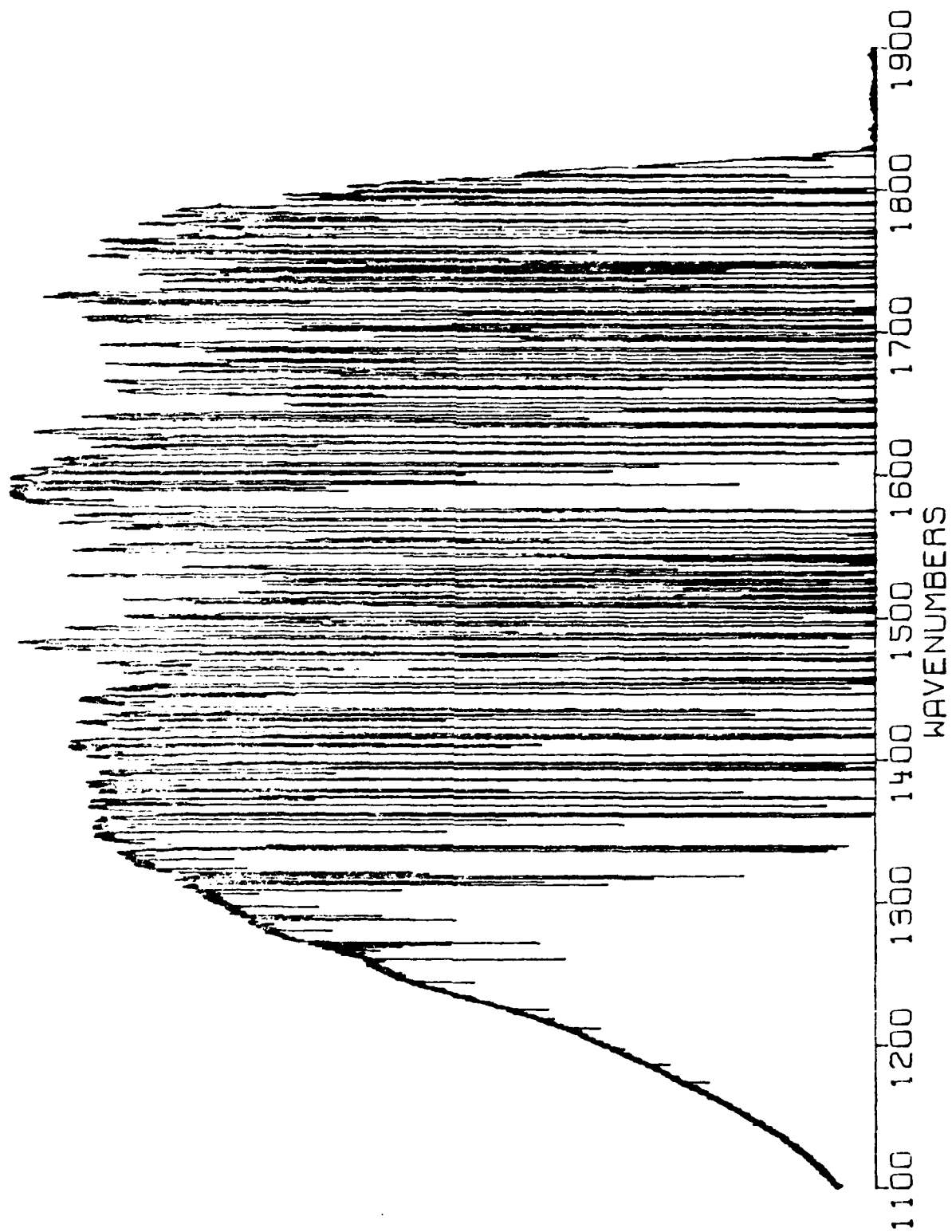


TABLE 2  
ABSORPTION DATA FOR NITRIC OXIDE

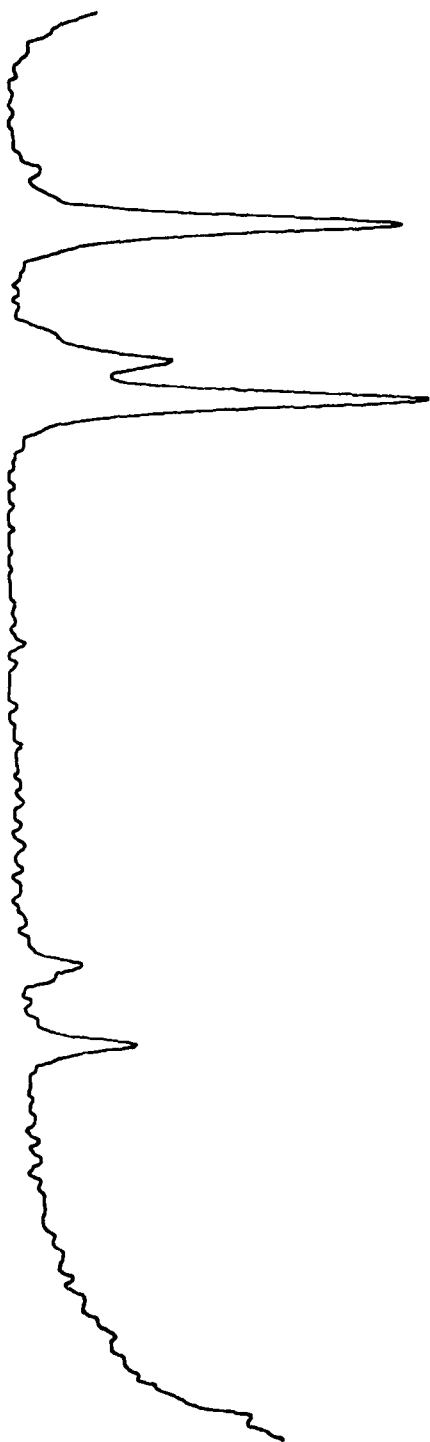
Band (Ref. 9)	Band Strength (Ref. 9) $\text{cm}^{-1}/\text{cm-atm}$	Line Identification (Ref. 10)	Line Position (Ref. 10)	Measured Effective Absorption Coefficient ( $\text{Torr}^{-1}$ )	Estimated Detection Limit (At 200 Torr Total Pressure)	Inteferring Species
1 - 0 $2\pi_{1/2}$	128	P(15/2)	1850.1757	$39.88 \pm 1.95$	$\approx 1.3 \text{ ppm}$	$\text{H}_2\text{O}$ $\text{CO}_2$
		P(13/2)	1853.7417	36.86		
		P(11/2)	1857.2736	37.07		

FIGURE 17 WATER VAPOR ABSORPTION - 1100  $\text{cm}^{-1}$  TO 1850  $\text{cm}^{-1}$



spectrum was obtained using the HgCdlc half of the "sandwich" detector and the interferometer fitted with the  $\text{Fe}_2\text{O}_3\text{-CaF}_2$  beamsplitter. The cutoff of signal near  $1100\text{ cm}^{-1}$  is due to the  $\text{CaF}_2$  transmission while the cutoff near  $1850\text{ cm}^{-1}$  is due to the transmission through the InSb part of the "sandwich". From Figure 17, it is clear that it will be difficult to observe  $\text{NO}_2$  absorption in this region; however, there is a small "window" in the water vapor centered at  $1586\text{ cm}^{-1}$  which is shown in Figure 18. Figure 19 shows the absorption in this region due to 50 ppm  $\text{NO}_2$  in 150 torr  $\text{N}_2$  and indicates that it should be possible to use this region to detect  $\text{NO}_2$ . An alternative band which could be used is the  $\nu_1 + \nu_3$  band of  $\text{NO}_2$  centered near  $2906\text{ cm}^{-1}$ . This band is free of interfering species; however, the band strength is only  $17\text{ cm}^{-1}/\text{cm-atm}$  (average of measurements [10]) and hence will yield a higher detection limit.

Since the CO spectrum is well known, only mention of the interference free lines will be given here. In the fundamental band, the P(3), P(2), P(1), and R(0) lines were selected for being free from interference by either  $\text{CO}_2$  or  $\text{N}_2\text{O}$  lines while in the first overtone, all lines were considered essentially interference free.



IR ABSORPTION IN THE  
 NO<sub>2</sub> REGION DUE TO  
 WATER VAPOR IN THE  
 SPECTROMETER ENVIRONMENT.

FIGURE 18 WATER VAPOR WINDOW - 1578  $\text{cm}^{-1}$  TO 1594  $\text{cm}^{-1}$

1578	1580	1582	1584	1586	1588	1590	1592	1594
WAVENUMBERS								

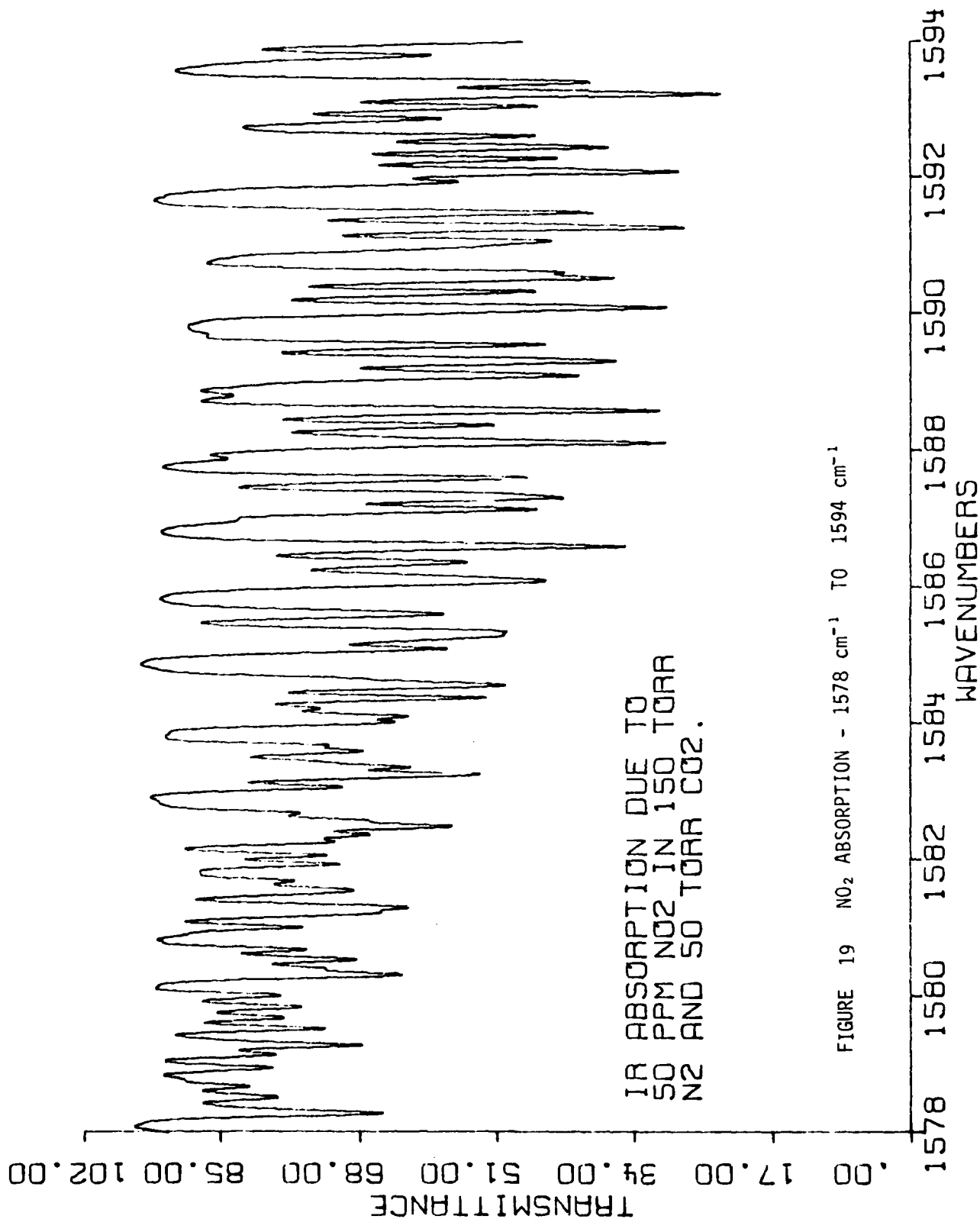


FIGURE 19 NO<sub>2</sub> ABSORPTION - 1578 cm<sup>-1</sup> TO 1594 cm<sup>-1</sup>

SECTION IV  
CALIBRATION PROCEDURE FOR IMPURITY  
CONCENTRATION

The easiest measured quantity that can be related to the partial pressure of a particular species is the transmittance of the gas at one of the absorbing wavelengths. If radiation from a source passes through the gas, the transmittance of the gas can be written

$$T(\nu) = 100\% \times \frac{I(\nu)}{I_0(\nu)} \quad (27)$$

where  $I(\nu)$  is the intensity of the radiation reaching the detector after passing through the gas, and  $I_0(\nu)$  is the intensity of the radiation reaching the detector when no gas is present. Theoretically, this can be related to the partial pressure of the absorber by

$$T(\nu) = 100\% \times \int_{-\infty}^{\infty} F(\nu-\nu') \cdot \exp\{-p \cdot x \cdot k(\nu')\} d\nu'. \quad (28)$$

In equation (28),  $p$  is the partial pressure of the absorber,  $x$  is the path-length over which the absorption occurs,  $k(\nu')$  is the absorption coefficient for the particular species as a function of wavenumber (or wavelength), and  $F(\nu-\nu')$  is the spectrometer bandpass function, normalized according to

$$\int_{-\infty}^{\infty} F(\nu) d\nu = 1. \quad (29)$$

If the spectrometer bandpass function is much "narrower" than the width of a spectral line,  $F(\nu-\nu')$  in equation (28) goes over to a delta function and the measured transmittance is just

$$T(\nu) = 100\% \times \exp\{-p \cdot x \cdot k(\nu)\}. \quad (30)$$

In this case, if one knows the absorption coefficient and the pathlength, the partial pressure can be calculated directly.

Unfortunately, the situation that exists when samples are analyzed with the White cell-FTS system is not so simple. The gas samples are normally at pressures of 100 torr or less which results in spectral linewidths on the order of  $0.01 \text{ cm}^{-1}$  (FWHM) or less, while the best instrument resolution is on or order of  $0.06 \text{ cm}^{-1}$ . Under these conditions the functional dependence of the transmittance on the partial pressure of the species becomes more complex. The simplest approach to solving this problem is to use calibration curves to relate the measured transmittance to the partial pressure of the species. In this procedure, a series of spectra are taken of gas mixes which contain known amounts of the species of interest and a calibration curve is constructed for each absorption line of each species. Then for a particular absorption line, one can write

$$T_k = A_k(p) \quad (31)$$

where the index  $k$  is used to indicate a particular line and  $A_k$  is the particular function that describes the transmittance of that line. This was the procedure initially chosen for calibration of the White-cell FTS system. The difficulty with using the aforementioned calibration procedure lies in the dependence of the function  $A_k$  on the other system parameters. For example, if the resolution of the spectrometer is changed, a new set of  $A_k$ 's must be generated for each new resolution setting. More important however,  $A_k$  is strongly dependent on the background gas pressure and weakly dependent on the composition of the background gas. Thus a separate set of calibration curves would have to be constructed for each total pressure run in the EBCC system or in the TEA laser experiment,



and for each gas mix chosen. For an experiment such as the EBCC system or the TEA laser, where one would like to vary these parameters at will, producing calibration data becomes exceedingly time consuming. An alternate calibration procedure, though perhaps less accurate, is to work directly with equation (28) to interpolate and extrapolate a manageable amount of calibration data. This has been the procedure adopted for the White cell-FTS system.

To see how equation (28) depends on the background pressure and gas mix, one needs to consider the absorption coefficient  $k(\nu)$ . For an isolated spectral line,  $k(\nu)$  can be written [11]

$$k(\nu) = \frac{S}{\alpha_D} \left( \frac{\ln 2}{\pi} \right)^{1/2} V(w, y) \quad (32)$$

where  $V(w, y)$  is the Voigt function given by

$$V(w, y) = \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-t^2) dt}{y^2 + (w-t)^2} \quad (33)$$

In equation (32),  $S$  is the integrated line strength and  $\alpha_D$  is the Doppler half-width of the line given by

$$\alpha_D = \nu_0 \left( \frac{2kT \ln 2}{Mc^2} \right)^{1/2} \quad (34)$$

where  $\nu_0$  is the wavenumber of the line,  $k$  is Boltzmann's constant,  $T$  is the gas temperature in Kelvin.  $M$  is the mass of the molecule, and  $c$  is the speed of light. In equations (32) and (33),  $w$  and  $y$  are defined by

$$w = \frac{\nu - \nu_c}{\alpha_D} (\ln 2)^{1/2} \quad (35)$$

and

$$y = \frac{\alpha_L}{\alpha_D} \quad (36)$$

where  $\nu$  is the wavenumber at which  $k(\nu)$  is desired,  $\nu_0$  and  $\alpha_D$  are as before, and  $\alpha_L$  is the Lorentz half-width of the line. The Lorentz width is made up of two components, the natural width  $\alpha_N$  and the collision width  $\alpha_C$ . For the range of pressures studied here,  $\alpha_N \ll \alpha_C$  so that for purposes of this study  $\alpha_L = \alpha_C$ . The collision half-width of the line is given by

$$\alpha_C = \sum_i \gamma_i p_i \quad (37)$$

where  $\gamma_i$  is the line broadening coefficient for the line under study, broadened by the  $i^{\text{th}}$  component in the gas mixture and  $p_i$  is the partial pressure of the  $i^{\text{th}}$  component. From equation (37) it can be seen that the collision half-width, and hence the absorption coefficient  $k(\nu)$ , depend on the total pressure of the gas and the particular species present. To use equation (28) to calculate partial pressures one must therefore know the line strength  $S$  of the particular line, the molecular weight of the absorbing species, and the broadening coefficients for each major species present in the gas mix. In addition, the partial pressures of the major components of the gas mix must also be known.

Since most of the data mentioned in the previous paragraph could be obtained from the open literature, one possible calibration scheme would consist of gathering the existing data and calculating the partial pressures of the major species directly. Since it was desired to develop a calibration scheme consistent with the calibration data that had already been obtained, a somewhat different scheme was chosen. It was found in the calculations that errors in the assumed widths of the lines were of less importance than errors in the individual line strengths. In addition, measurement

of broadening coefficients would require many additional calibration measurements which would be quite time consuming. So for these reasons, the calibration scheme chosen involved using broadening coefficients from the open literature along with line strengths calculated from the calibration data. Before any of this could be implemented, a number of computer codes had to be developed in order to evaluate equation (28). To calculate the Voigt function in equation (32) a code due to Armstrong [11] was modified slightly and implemented. This function subprogram is called VOIGT. To evaluate equation (28) a code called FOLD1 was written which uses Simpson's one-third rule to evaluate the integral. The step size in FOLD1 is automatically adjusted to handle variations in line width and the limits on the integral are adjusted in accordance with the instrument resolution. The spectrometer bandpass function is supplied by a function subprogram called BPASS1 which was written especially for this FTS system. To calculate the strength of a particular line it was necessary to "solve" equation (28) for  $S$  (from equation (32)) given a particular line center transmittance, partial pressure, and line width. For this, a code called SEEKER2 was written which solves equation (28) for  $S$  by an iterative procedure. Finally, after the line strengths were estimated a code was needed to solve equation (28) for  $p$  given  $k(\nu_0)$  and  $T(\nu_0)$  for an "unknown" gas sample. A code called SEEKER1 was written for this purpose and like SEEKER2 uses an iterative approach. Data arrived at for use in measuring minor species in the White cell FTS system is presented in Tables 3 through 7. The lines in the tables were primarily selected because they are free from interference by strong water vapor lines, hot bands of  $\text{CO}_2$ , and lines of other minor species. Whenever possible, two bands of the same molecule were used (weak and strong) to increase the dynamic range of the measurement and further reduce the chances of interference. The line strengths given in the third column of each table were arrived at by

TABLE 3

LINE PARAMETERS FOR SELECTED INTERFERENCE-FREE LINES OF THE  $^{12}\text{C}^{16}\text{O}$  FUNDAMENTAL

Line Designation	Line Position <sup>a</sup> ( $\text{cm}^{-1}$ )	Line Strength ( $\text{cm}^{-2} \text{ atm}^{-1}$ @296°) This Work <sup>b</sup> Literature Value <sup>c</sup>	Line Broadening Coefficients ( $\text{cm}^{-1} \text{ atm}^{-1}$ )			
			Self <sup>d</sup>	$\text{CO}_2$ <sup>e</sup>	$\text{N}_2$ <sup>d</sup>	He <sup>d</sup>
P(3)	2131.6320	--	.0785	.0967	.0721	.0466
P(2)	2135.5466	--	.0831	.1026	.0776	.0468
P(1)	2139.4265	--	.0877	.1118	.0812	.0479
R(0)	2147.0816	--	.0877	.1118	.0812	.0479

## NOTES FOR TABLE 3

- From Reference 1
- For the  $\text{CO}$  Fundamental, it was felt that the literature values were far superior to any that could be measured in this experiment
- Calculated from data of Reference 12. Uncertainty is probably less than  $\pm 5\%$
- From Reference 13
- From Reference 14

TABLE 4

LINE PARAMETERS FOR SELECTED LINES OF THE  $^{12}\text{C}^{16}\text{O}$  1st OVERTONE

Line Designation	Line Position <sup>a</sup> ( $\text{cm}^{-1}$ )	Line Strength ( $\text{cm}^{-2} \text{ atm}^{-1}$ @296°)		Line Broadening Coefficients ( $\text{cm}^{-1} \text{ atm}^{-1}$ )				
		This Work <sup>b</sup>	Literature Values <sup>c</sup>	Self <sup>d</sup>	$\text{CO}_2$ <sup>d</sup>	$\text{N}_2$ <sup>d</sup>	He <sup>e</sup>	
P(8)	4227.3544	6.758E-02	6.832E-02	.0682	.0782	.0635	.0455	
P(7)	4231.6853	6.904E-02	6.984E-02	.0695	.0813	.0630	.0455	
P(6)	4235.9474	6.781E-02	6.859E-02	.0711	.0848	.0652	.0458	
R(6)	4285.0093	8.506E-02	8.604E-02	.0695	.0813	.0640	.0455	
R(7)	4288.2901	8.578E-02	8.673E-02	.0682	.0782	.0635	.0455	
R(8)	4291.4998	8.359E-02	8.455E-02	.0670	.0755	.0630	.0455	

## NOTES FOR TABLE 4

- From Reference 1
- Estimated uncertainty is  $\pm 5\%$ . Bandstrength calculated is  $2.27 \pm .11 \text{ cm}^{-2} \text{ atm}^{-1}$  at  $300^\circ\text{K}$
- Relative strengths calculated from Reference 12, but scaled to yield band strength used in Reference 15 ie.  $2.291 \text{ cm}^{-2} \text{ atm}^{-1}$  at  $300^\circ\text{K}$ . Uncertainty is probably less than 5%
- From Reference 14
- From Reference 13

TABLE 5

LINE PARAMETERS FOR SELECTED INTERFERENCE FREE LINES OF THE  $^{14}\text{N}^{16}\text{O}$  FUNDAMENTAL

Line Designation	Line Position <sup>a</sup> ( $\text{cm}^{-1}$ )	Line Strength ( $\text{cm}^{-2} \text{ atm}^{-1}$ @296°)		Line Broadening Coefficients ( $\text{cm}^{-1} \text{ atm}^{-1}$ )			
		This Work <sup>b</sup>	Literature Value <sup>c</sup>	Self <sup>d</sup>	$\text{CO}_2\text{e}$	$\text{N}_2\text{f}$	Hee
$(^2\pi_{3/2})$							
P(15/2)	1850.1757	2.684	2.53	.0589	.0683	.0589	.0405
P(13/2)	1853.7417	2.624	2.47	.0583	.0676	.0583	.0401
P(11/2)	1857.2736	2.468	2.32	.0595	.0690	.0595	.0409
P(9/2)	1860.7713	2.205	2.07	.0611	.0709	.0611	.0420

## NOTES FOR TABLE 5

- From Reference 10
- Estimated uncertainty is  $\pm 2.4\%$ . Bandstrength calculated is  $127 \pm 3 \text{ cm}^{-2} \text{ atm}^{-1}$  at  $300^\circ\text{K}$
- From Reference 16 Bandstrength given is  $122 \pm 6 \text{ cm}^{-2} \text{ atm}^{-1}$  at  $300^\circ\text{K}$  (an uncertainty of approx.  $\pm 5\%$ )
- From Reference 16 (average value of  $^2\pi_{1/2}$  and  $^2\pi_{3/2}$  states)
- J dependence is assumed to be the same as Reference 16, but absolute value results from multiplying  $\gamma$  (self) values from Reference 16 by  $\gamma(x)/\gamma(\text{self})$  from Reference 8
- Assumed to be the same as  $\gamma$  (self) from Reference 16

TABLE 6

LINE PARAMETERS FOR SELECTED INTERFERENCE-FREE LINES OF THE  $\nu_3$  BAND OF  $^{14}\text{N}_2$   $^{16}\text{O}$ 

Line Designation	Line Position <sup>a</sup> ( $\text{cm}^{-1}$ )	Line Strength ( $\text{cm}^{-2} \text{ atm}^{-1}$ @ 296°)		Line Broadening Coefficients ( $\text{cm}^{-1} \text{ atm}^{-1}$ )			
		This Work <sup>b</sup>	Literature Value <sup>c</sup>	Self <sup>d</sup>	$\text{CO}_2$ e	$\text{N}_2$ f	He <sup>g</sup>
P(37)	2188.1898	5.192	5.07	.0713	.0673	.0681	.0508
P(36)	2189.2734	5.873	5.73	.0720	.0666	.0680	.0507
P(35)	2190.3502	6.610	6.45	.0728	.0659	.0679	.0506

## NOTES FOR TABLE 6

53

- From Reference 8
- Estimated uncertainty is  $\pm 10\%$ . Calculated bandstrength is  $1190 \pm 107 \text{ cm}^{-2} \text{ atm}^{-1}$  at  $300^\circ\text{K}$
- From Reference 18. Uncertainty given is about  $\pm 2.6\%$ . Bandstrength is  $1173 \pm 30 \text{ cm}^{-2} \text{ atm}^{-1}$  at  $300^\circ\text{K}$
- The J-dependence of Reference 19 was used but values were normalized so that P(35) coefficient agreed with that of Reference 20. Reference 20 value is corrected for temperature dependence by  $(296/300)^{1/2}$
- The J-dependence of Reference 19 was used but values were normalized to the  $|m|=6$  value of Reference 21 for  $\gamma(\text{CO}_2)$  at  $J=6$
- The values from Reference 19 were multiplied by 0.9 to bring them in line with the data from Reference 21 and 22
- Same as note e except values were normalized to the  $\gamma(\text{He})$  value of Reference 21

TABLE 7

LINE PARAMETERS FOR SELECTED INTERFERENCE-FREE LINES OF THE  $2\nu_1$  BAND OF  $^{14}\text{N}_2$   $^{16}\text{O}$ 

Line Designation <sup>a</sup>	Line Position <sup>b</sup> ( $\text{cm}^{-1}$ )	Line Strength ( $\text{cm}^{-2} \text{ atm}^{-1}$ @296°)		Line Broadening Coefficients ( $\text{cm}^{-1} \text{ atm}^{-1}$ )			
		This Work <sup>c</sup>	Literature Value <sup>d</sup>	Self <sup>e</sup>	$\text{CO}_2$ <sup>f</sup>	$\text{N}_2$ <sup>g</sup>	He <sup>h</sup>
P(16)	2549.1178	.5742	.5566	.0933	.0860	.0756	.0563
P(15)	2550.0573	.5745	.5569	.0941	.0860	.0770	.0573
P(14)	2550.9901	.5700	.5700	.5526	.0950	.0860	.0573
R(14)	2575.0912	.6107	.5920	.0941	.0860	.0762	.0568
R(15)	2575.8199	.6128	.5941	.0933	.0860	.0756	.0563
R(16)	2576.5418	.6100	.5914	.0926	.0860	.0749	.0553

## NOTES FOR TABLE 7

- For brevity, only data for six strongest lines is presented here. Data also exists for P(17), P(13), P(12), R(12), R(13), and R(17)
- From Reference 8
- Estimated uncertainty is  $\pm 5\%$ . Calculated bandstrength is  $30.3 \pm 1.5 \text{ cm}^{-2} \text{ atm}^{-1}$  at  $300^\circ\text{K}$
- Relative strengths are from Reference 23. Bandstrength is from Table 14 of Reference 7. Bandstrength is  $29.4 \pm 1.5 \text{ cm}^{-2} \text{ atm}^{-1}$  at  $300^\circ\text{K}$
- From Reference 20 scaled to  $296^\circ$  by  $(296/300)^{1/2}$
- J-dependence of Reference 20 with the values normalized to the  $|m|=6$  value for  $\gamma(\text{CO}_2)$  of Reference 21.
- See Note f of Table III-6
- See Note g of Table III-6



first taking the averages of the strengths calculated from each calibration curve by SEEKER2, then "smoothing" the values to fit theoretical relative intensities at 296°K. This "smoothing" was done by first calculating a band strength from each line strength using theoretical relative intensities. Then an average band strength and its standard deviation were calculated and a set of line strength derived from this average band strength using the theoretical relative intensities. These final line strengths were taken as the "smoothed" values. The data in Tables 3 through 7 is now on computer cards and used by a driving program called TRACER. TRACER uses SEEKER1 and specific line parameter data to arrive at partial pressures of CO, N<sub>2</sub>O, and/or NO in a given sample of gas. A listing of TRACER is given in Appendix III.

## SECTION V

### IMPURITIES IN CO<sub>2</sub> LASER DISCHARGES

Gas samples from the electron beam closed cycle laser and from a TEA laser were analyzed to determine the extent of dissociation and gas chemical effects in the discharge. Before discussing the results in general, the results from two gas samples will be discussed in detail.

Gas samples from the EBCC loop were always taken before and after running the E-beam to insure that the gas was initially clean. Following irradiation, the samples were introduced into the absorption cell and their spectra taken. Changes in the gas were then noted by comparing the spectra of the pre-irradiated gas with the irradiated sample. The first irradiated sample of gas was from approximately a two hour E-beam run, while the second irradiated sample was taken after about a seven hour run. In both cases, the pre-irradiated samples showed only the spectra expected from the 1:2:3 mix. For the two hour irradiated sample, the only difference from the pre-irradiated gas was the presence of CO lines in the irradiated sample spectrum. The seven hour irradiated sample, however, showed significant changes. For example, Figure 20 shows a portion of the absorption spectrum of the pre-irradiated gas while Figure 21 shows the same region of the spectrum of the irradiated sample. In the irradiated sample spectrum both N<sub>2</sub>O and CO lines can be clearly seen in addition to the CO<sub>2</sub> lines from the 1:2:3 mix. Figure 22 shows a calibration spectrum of 38 ppm N<sub>2</sub>O in the 1:2:3 mix and indicates the order of magnitude of the N<sub>2</sub>O absorption. In addition to the N<sub>2</sub>O lines and the CO lines, lines due to NO were also seen in the irradiated sample which were not seen in the pre-irradiated gas. Figure 23 shows a portion of the irradiated sample spectrum showing the NO lines, while Figure 24 shows a typical calibration spectrum.

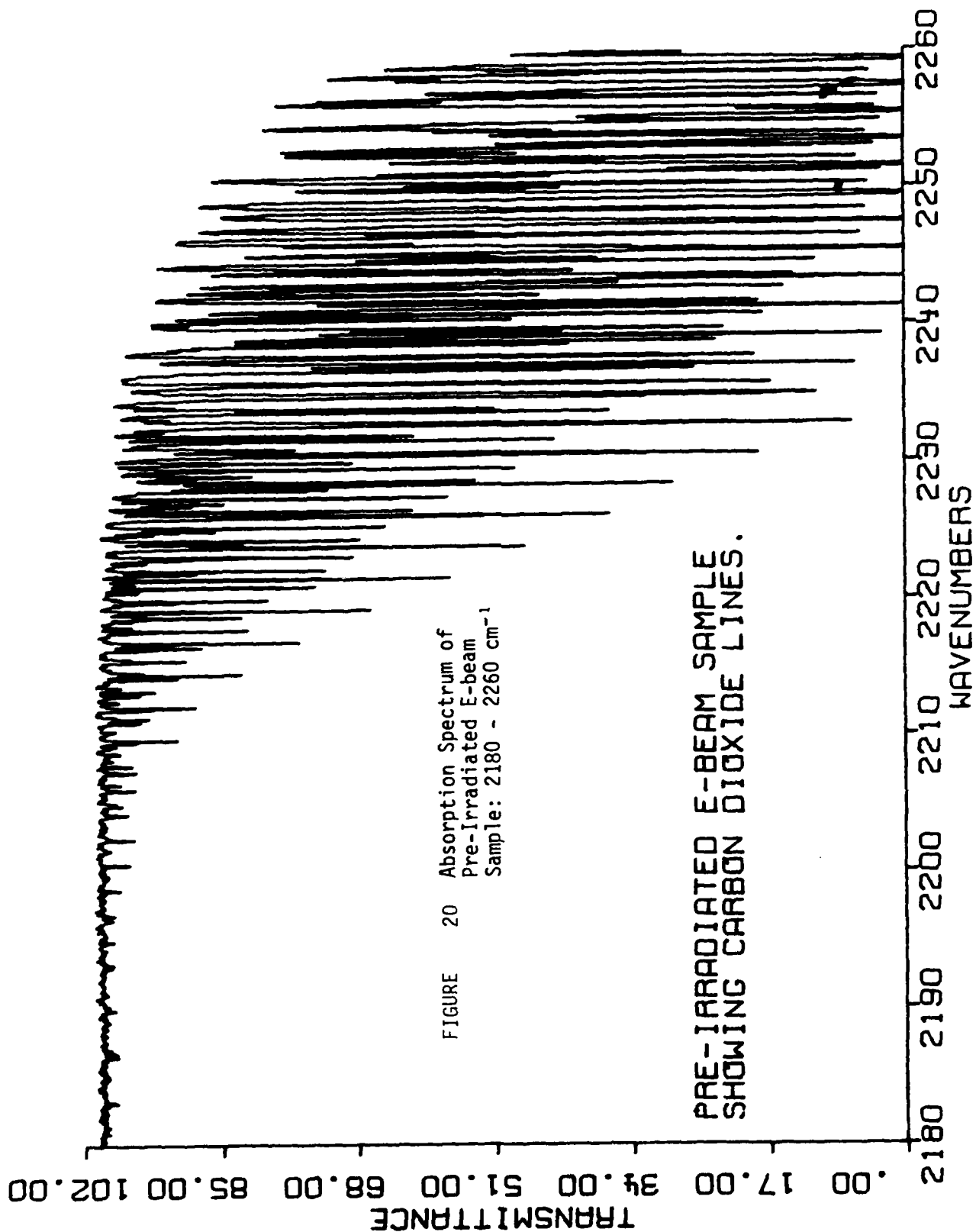
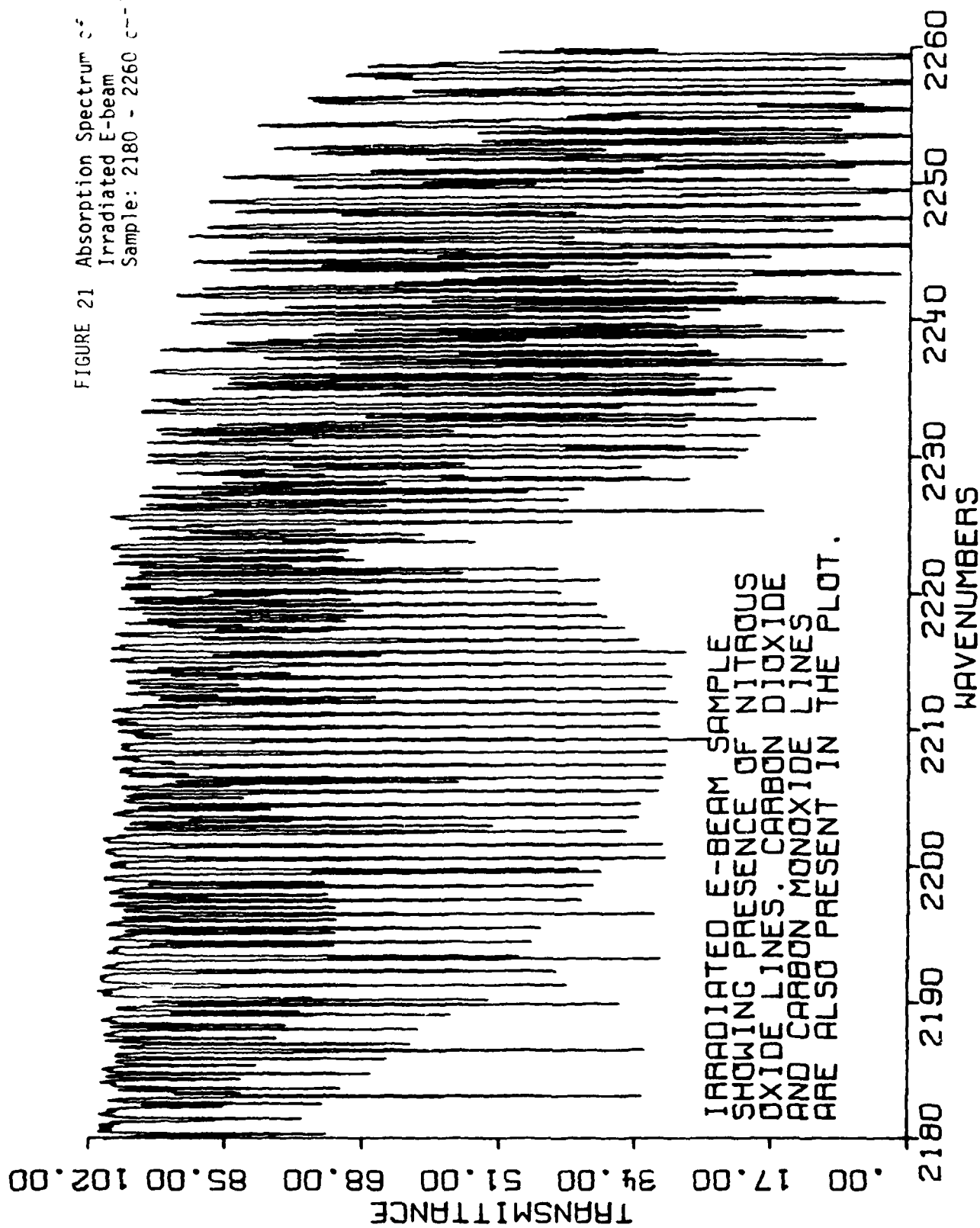
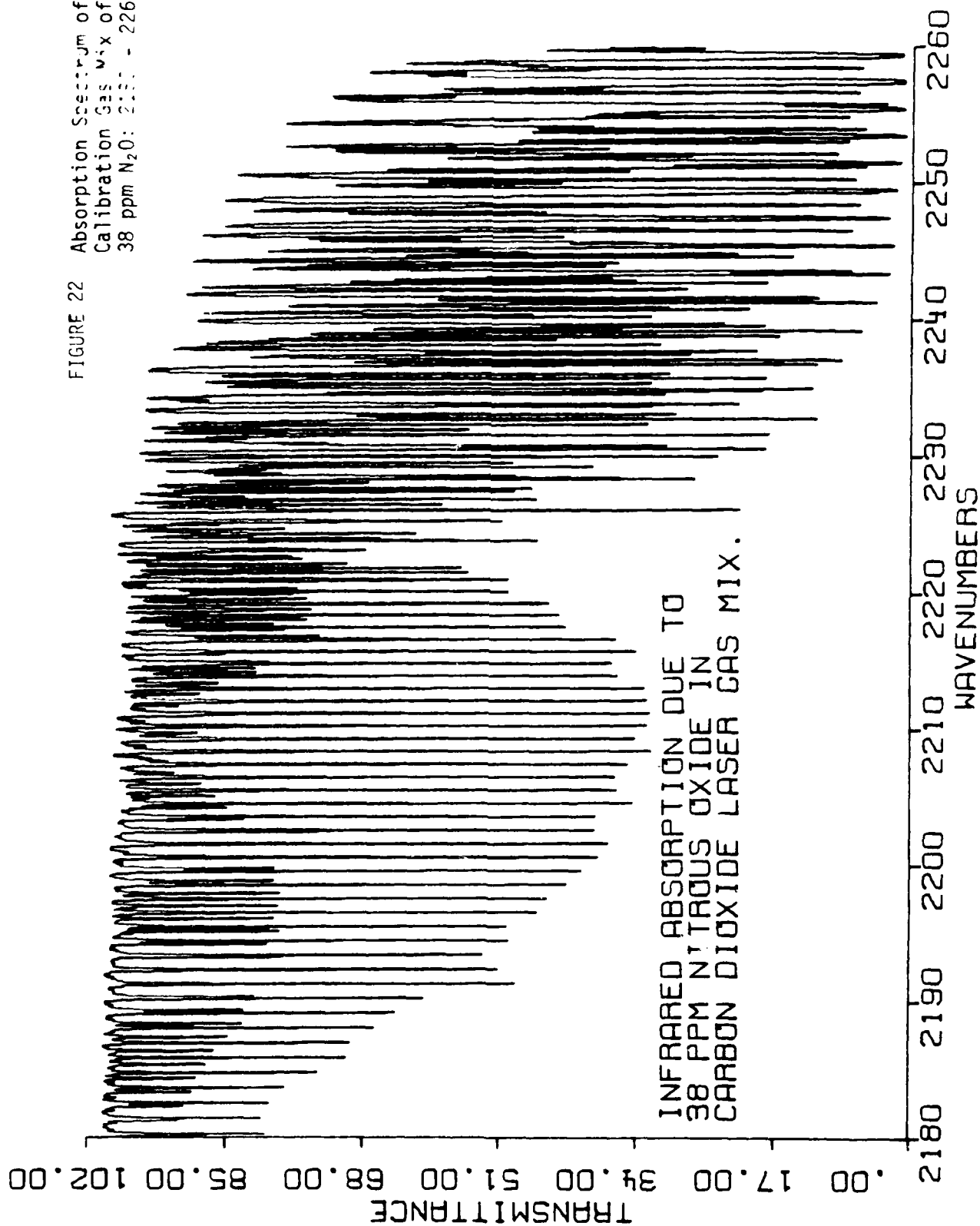


FIGURE 21 Absorption Spectrum of  
Irradiated E-beam  
Sample: 2180 - 2260  $\text{cm}^{-1}$





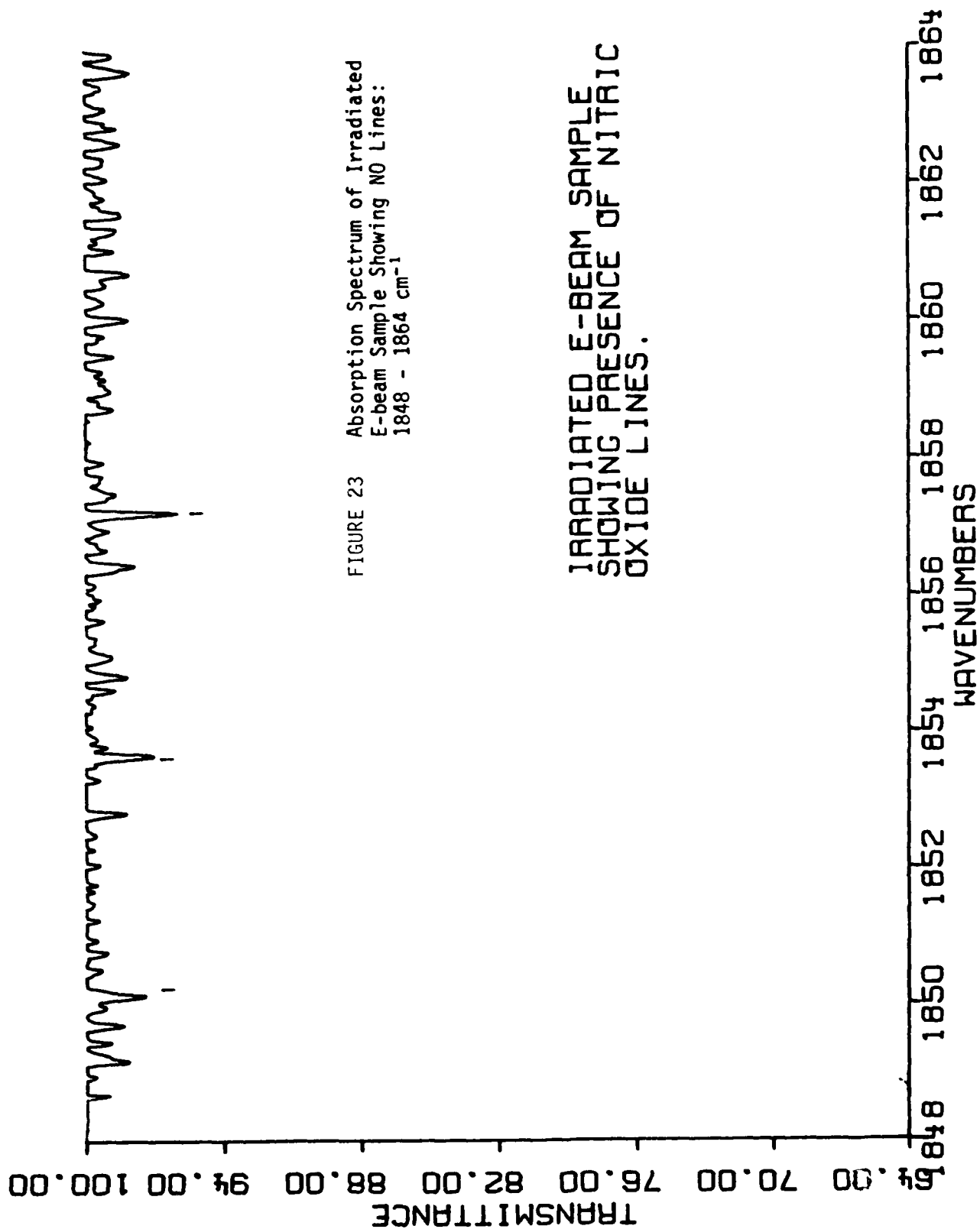


FIGURE 23 Absorption Spectrum of Irradiated  
E-beam Sample Showing NO Lines:  
1848 - 1864  $\text{cm}^{-1}$

IRRADIATED E-BEAM SAMPLE  
SHOWING PRESENCE OF NITRIC  
OXIDE LINES.

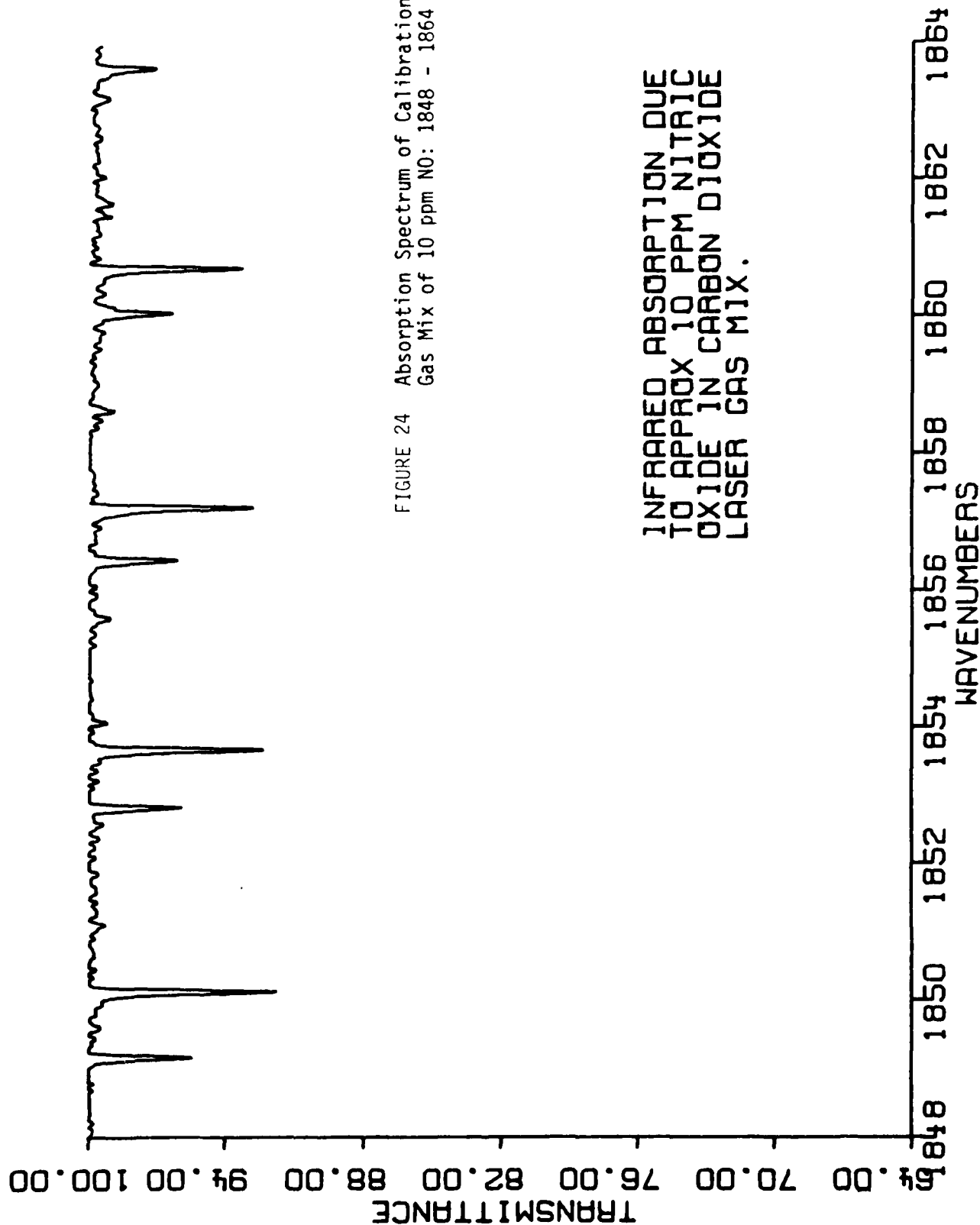


FIGURE 24 Absorption Spectrum of Calibration  
Gas Mix of 10 ppm NO: 1848 - 1864  $\text{cm}^{-1}$

INFRARED ABSORPTION DUE  
TO APPROX 10 PPM NITRIC  
OXIDE IN CARBON DIOXIDE  
LASER GAS MIX.

Table 8 summarizes the results of the two data sets and includes estimates of the concentrations of the species present. No unusual spectral features were seen in either of the samples.

Measurements of the selected trace constituents in TEA laser gases have been obtained. The laser used is a Molelectron model T250 run at about one-half atmosphere (actually a CO<sub>2</sub> TE laser). In the experiment, the laser is run sealed off for a specific number of pulses, then a gas sample is taken and analyzed. The limit on the number of pulses that can be run is determined by the onset of repeated arcing of the laser. Figure 25 shows the results obtained for one series of data runs of the laser. The gas mix used was made up of 260 torr of a 1:2:3 mix (CO<sub>2</sub>:N<sub>2</sub>:He) and 40 torr of H<sub>2</sub>. Repetition rate for the laser was kept low to reduce gas heating and was about 0.75 Hz. Pulse width was roughly 1 μsec and voltage was about 25Kv. In all of the TE laser results, the predominant NO<sub>x</sub> compound is NO, while in most of the EBCC data (at atmospheric pressure) the predominant species is N<sub>2</sub>O. The only exception to this was some EBCC data taken after only one-half hour irradiation of the gas. In this very short irradiation, no N<sub>2</sub>O lines were seen while the weaker NO lines are measureable. Thus, it appears that except for very short runs of the E-beam, the predominant nitrogen oxide is N<sub>2</sub>O while in all the TE laser samples taken so far, NO is predominant. In all cases, no NO<sub>2</sub> could be detected.

A systematic study was performed of gas decomposition in the EBCC discharge and the effect of hydrogen and oxygen as gas additives. The results were presented at the 1979 Gaseous Electronics Conference [24]. For all the results presented here, the laser was operated with 250 Torr of CO<sub>2</sub> and 500 Torr of N<sub>2</sub> for a period of one hour before the gas was analyzed.



TABLE 8  
ESTIMATES OF MINOR SPECIES CONCENTRATIONS IN EBCC GAS SAMPLES

Species	Estimated Concentration (ppm)	
	2 Hours RUN	7 Hour RUN
CO	120 ± 10	200 ± 10
N <sub>2</sub> O	< .8	47 ± 3
NO	< 1	5 ± 2
NO <sub>2</sub>	< 2	< 2

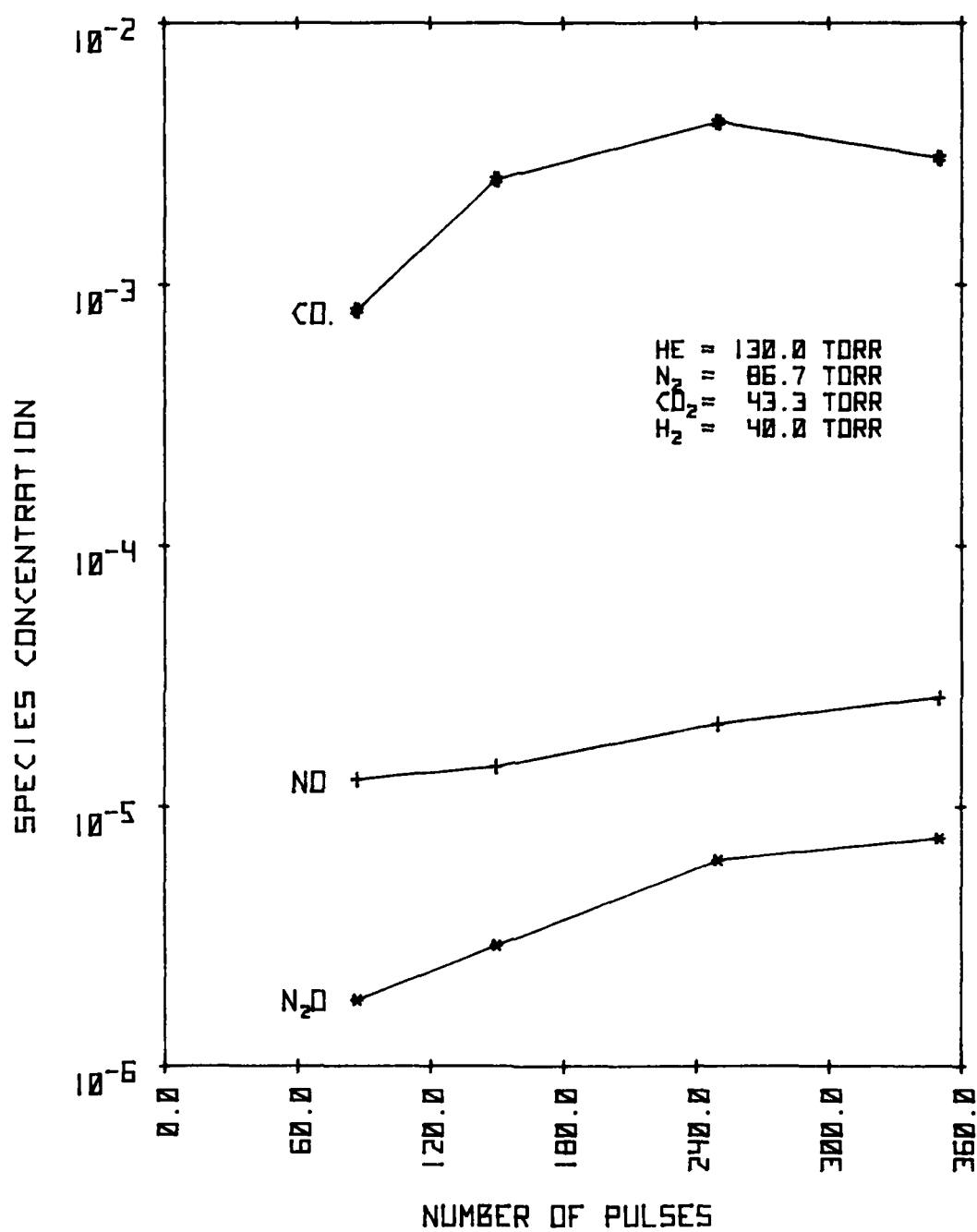


FIGURE 25 MINOR SPECIES BUILD UP IN A CO<sub>2</sub> TE LASER

With a pure  $N_2/CO_2$  gas mix the oxides of nitrogen built up to the 10 ppm (parts per million) range while the CO concentration was of the order of a few hundred ppm. On line absorption measurements with the tunable diode laser showed that the build up of CO was very rapid when the laser was initially turned on, and reached a stable value after a few hundred seconds.

This laser system has very good vacuum capabilities, whereas most other laser systems have larger vacuum leaks. A small amount of oxygen was added to the gas mix to simulate the more usual conditions. The results, shown in Figure 26, indicate an increase in both CO and the oxides of nitrogen. At a pressure of five Torr added oxygen, the concentration of CO,  $N_2O$ ,  $NO_2$  and NO are increased by factors of 8, 20, 12, and 6 respectively over the results obtained without added oxygen. Prior to the experiment, it was expected that the additional oxygen would react with CO to reform  $CO_2$  lowering the CO concentration. Instead the oxygen appears to enhance the formation of CO.

The effect of adding hydrogen was investigated since many  $CO_2$  systems now use gas mixtures containing hydrogen [25]. As shown in Figure 27, NO and  $NO_2$  concentrations decrease with added hydrogen. The behavior of  $N_2O$  might be explained by dissociation of  $HNO_2$  or  $HNO_3$  formed in the discharge from NO and  $NO_2$ . No  $HNO_3$  or  $HNO_2$  was observed in the gas mix, but wouldn't be expected in large quantities if their destruction to  $N_2O$  was rapid compared to their formation. The sensitivity to  $HNO_3$  detection was estimated at 10 ppm.

As hydrogen is added to the gas mix the concentrations of both CO and  $H_2O$  increase. This may be because the hydrogen reacts with the dissociatively produced oxygen to prevent the back reaction of CO to reform  $CO_2$ .

Finally hydrogen and oxygen were added together to the laser gas mix, with the results as shown in Figure 28. As before the concentration of NO and  $NO_2$  after one hour irradiation was smaller when hydrogen was added than

FIGURE 26 Effect of added oxygen on  
minor species concentration  
of an E B C SYSTEM

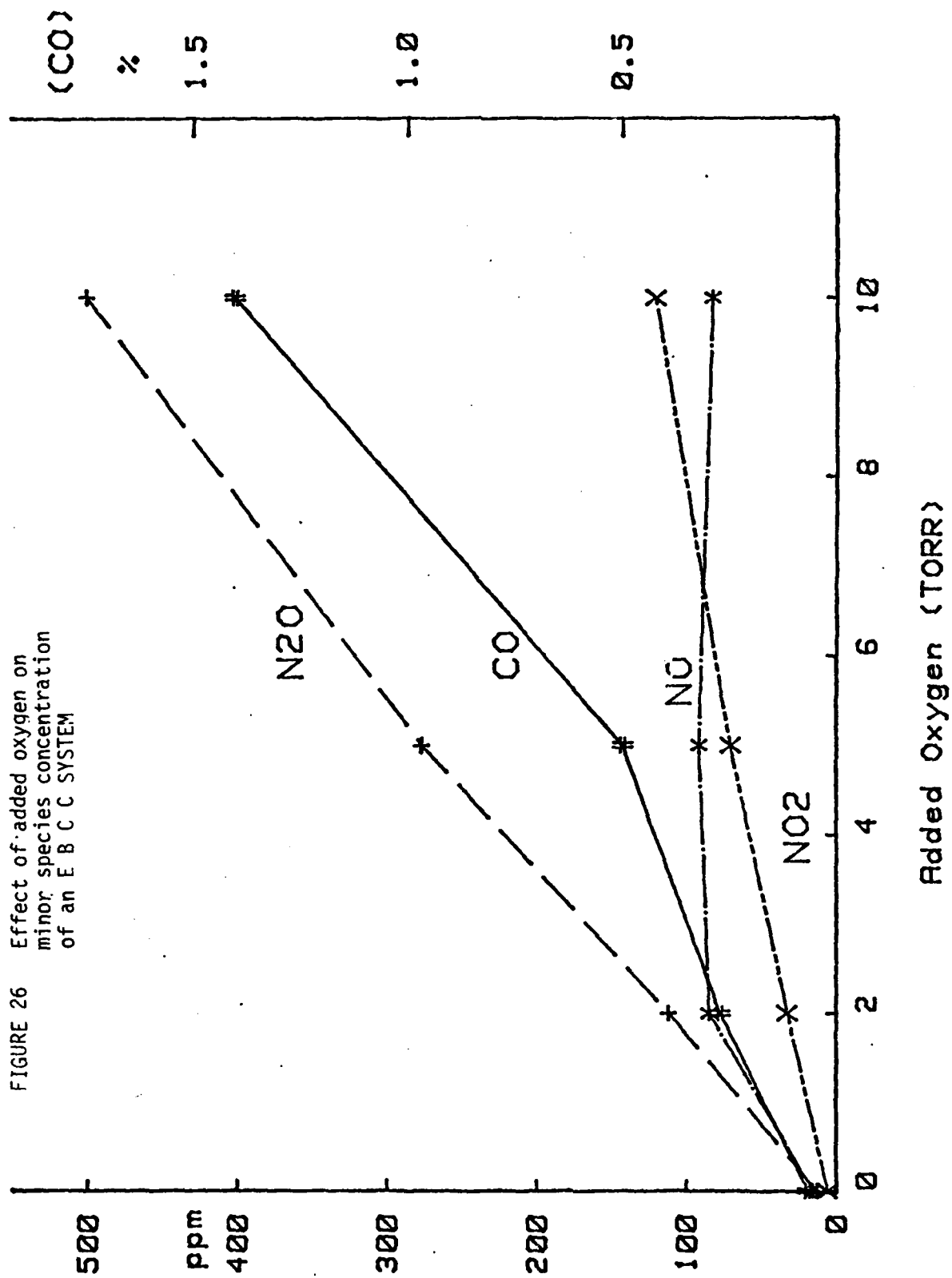


FIGURE 27

EFFECT OF HYDROGEN ON E.B.C.C. SYSTEM GAS  
COMPOSITION AFTER 1 HOUR IRRADIATION:  
OXYGEN FREE INITIAL GAS MIX.

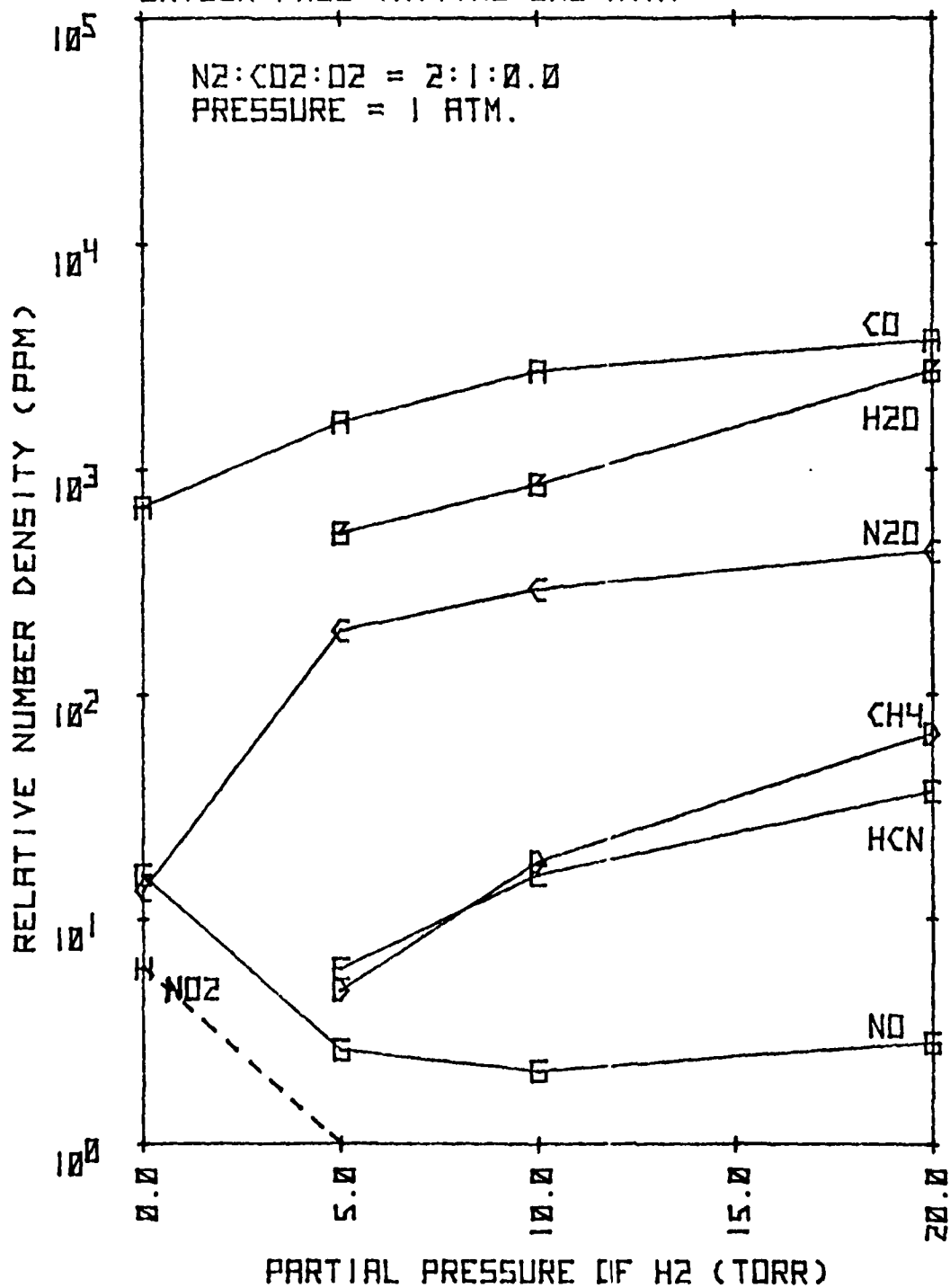
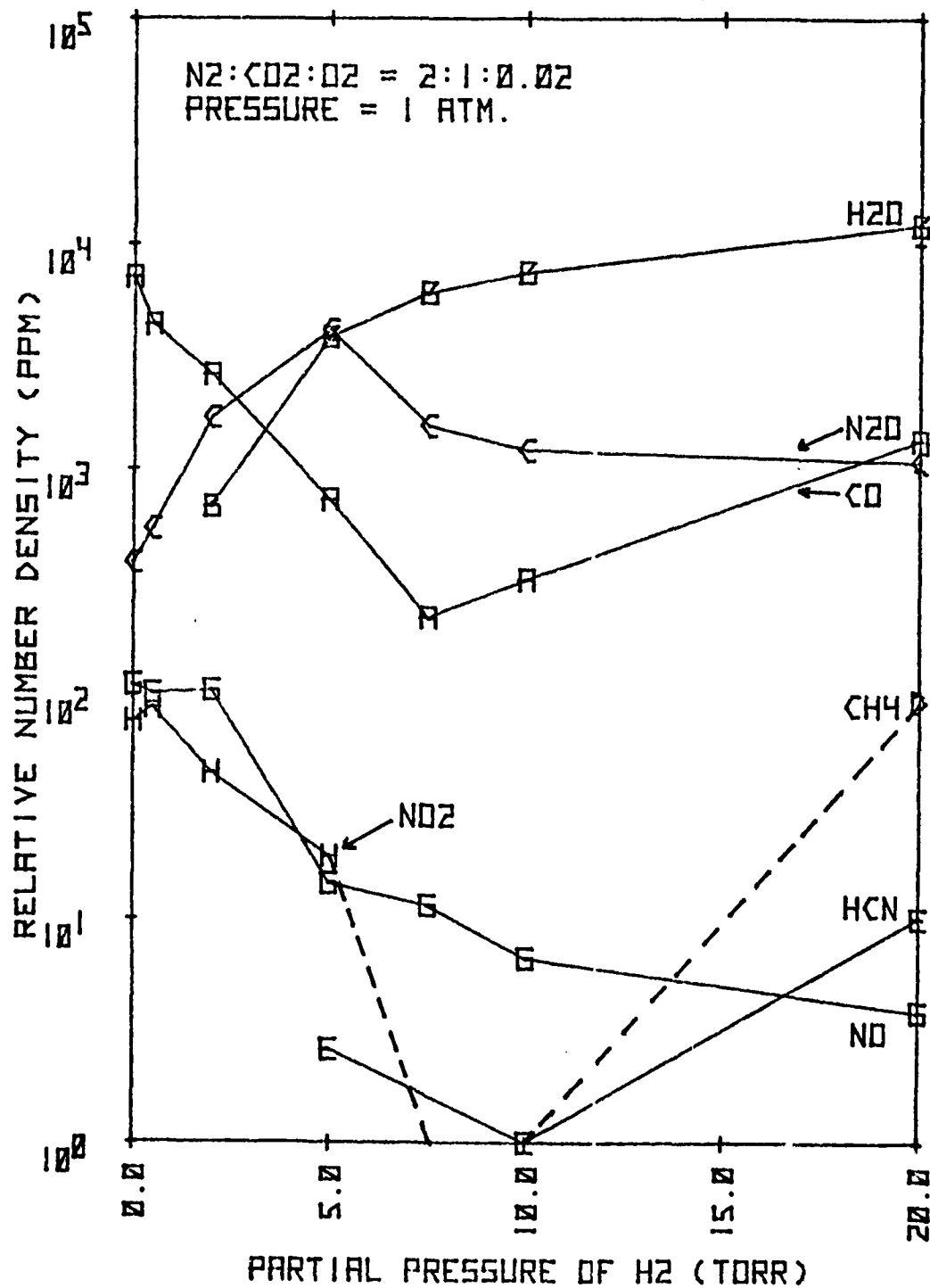


FIGURE 28

EFFECT OF HYDROGEN ON E.B.C.C. SYSTEM GAS  
COMPOSITION AFTER 1 HOUR IRRADIATION:  
5 TORR OXYGEN IN INITIAL GAS MIX.



when hydrogen was absent. However the concentration of NO, NO<sub>2</sub> and N<sub>2</sub>O is greater for a given amount of hydrogen when both hydrogen and oxygen were added than when hydrogen alone was added. The CO concentration drops to a level below that observed in the basic N<sub>2</sub>:CO<sub>2</sub> mix. To explain the behavior of CO two competing effects must be considered. The presence of H<sub>2</sub> lowers the concentration of discharge produced oxygen and tends to increase the CO level by preventing its back reaction of reform CO<sub>2</sub>. It also appears that H<sub>2</sub>O tends to reduce the CO concentration. The catalytic reaction of H<sub>2</sub>O with CO to form CO<sub>2</sub> has previously been observed. As in the previous case, CH<sub>4</sub> and HCN appear, but only at higher H<sub>2</sub> concentrations.

In conclusion, the addition of oxygen to the gas mix greatly increases the production of nitrogen oxides and carbon monoxide. The addition of hydrogen to an oxygen free gas mix produces water at ~10% of the H<sub>2</sub> concentration, increases the production of N<sub>2</sub>O and CO while decreasing NO and NO<sub>2</sub>.

The addition of hydrogen and a fixed quantity of oxygen to the gas mix produces water at 55% of the original H<sub>2</sub> concentration (up to twice the added O<sub>2</sub> concentration), increases the N<sub>2</sub>O production but decreases that of CO, NO, and NO<sub>2</sub>. When hydrogen was added to the mix, with or without oxygen, CH<sub>4</sub> and HCN were produced, but no HNO<sub>3</sub> or HNO<sub>2</sub> was detected in the irradiated gas mix.

## REFERENCES

1. Cole, A.R.H., Tables of Wave Numbers for the Calibration of Infrared Spectrometers, 2nd ed., Pergamon Press (1977).
2. Bell, John Robert, Introductory Fourier Transform Spectroscopy, Academic Press (1972).
3. Lawson, J.L. and Uhlenbeck, G.E., Threshold Signals, M.I.T. Radiation Laboratory Series Vol. 34, McGraw-Hill Book Company, Inc. (1950).
4. Marquardt, D.W., J. Soc. Ind. Appl. Math., 11, 431 (1963).
5. Bevington, P.R., Data Reduction and Error Analysis for the Physical Sciences, McGraw-Hill Book Company, 1969.
6. Treanor, C.E., Rich, J.W., and R.G. Rehm, J. Chem. Phys., 48, 1798 (1968).
7. McClatchey, et. al., "AFCRL Atmospheric Absorption Line Parameters Compilation," AFCRL-TR-73-0096 (26 Jan. 1973).
8. Amiot, C. and Guelachvili, G., "Extension of  $10^6$  Samples Fourier Spectrometry to the Indium Antimonide Region: Vibration-Rotation Bands of  $^{14}\text{N}_2$   $^{16}\text{O}$ : 3.5-5.5  $\mu\text{m}$  Region", J. Mol. Spec., 59, 171-190 (1976).
9. Young, L.G., "Compilation of Stratospheric Trace Gas Spectral Parameters", AFCRL-TR-76-0033 (15 Feb. 1976).
10. NO line positions were taken from a list supplied with the AFAPL/POD Tunable Diode Laser System. The measurements are from the Laboratoire De Spectronomie Moleculaire, Universite De Paris VI, however, it is not known if these line positions have been published.
11. Armstrong, B.H., "Spectrum Line Profiles: The Voight Function", J.Q.S.R.T., 18, 61 (1967).
12. Young, Lee A. and Eachus, James W., "Dipole Moment Function and Vibration Rotation Matrix Elements of CO", J. Chem. Phys., 44, 4195 (1966).
13. Draegert, D.A. and Williams, D., "Collisional Broadening of CO Absorption Lines by Foreign Gases", J. Opt. Soc. Am., 58, 1399 (1968).
14. Bouanich, J.P. and Brodbeck, C., "Mesures Des Largeurs et Des Deplacements Des Raies De La Bande  $0 \rightarrow 2$  De CO Autoperturbe et Perturbe Par  $\text{N}_2$ ,  $\text{O}_2$ ,  $\text{H}_2$ , HCL, NO, et  $\text{CO}_2$ ", J.Q.S.R.T., 13 (1973).



15. Chackerian, Jr., C., "Electric Dipole Moment Function of the  $X^1\Sigma^+$  State of CO: Vibration-Rotation Matrix Elements for Transitions of Gas Laser and Astrophysical Interest", J. Chem. Phys. 65, 4228 (1976).
16. Abels, L.L. and Shaw, J.H., "Widths and Strengths of Vibration-Rotation Lines in the Fundamental Band of Nitric Oxide", J. Mol. Spec., 20, 11 (1966).
17. French, I.P. and Arnold, Jr., T.E., "Linewidth of the  $J=1/2 \rightarrow 3/2$  Rotational Absorption in Nitric Oxide", J. Chem. Phys., 48, 5720 (1968).
18. Boissy, J.P., Valentin, A., Cardinet, Ph., Claude, M.L., and Henry A., "Line Intensities of the  $\nu_3$  Fundamental Band of Nitrous Oxide", J. Mol. Spec., 57, 391 (1975).
19. Toth, R.A., "Self-Broadened and  $N_2$  Broadened Linewidths of  $N_2O$ ", J. Mol. Spec., 40, 605 (1971).
20. Tejwani, G.D.T. and Veranasi, P., "Theoretical Line Widths in  $N_2O-N_2O$  and  $N_2O$ -Air Collisions", J.Q.S.R.T., 11, 1659 (1971).
21. French, I.P. and Arnold, Jr., T.E., "Foreign-Gas Broadening of the  $J=5 \rightarrow 6$  Rotational Transition of Nitrous Oxide", J. Mol. Spec., 27, 218 (1968).
22. Lowder, J.E., "Band Intensity and Line Half-Width Measurements in  $N_2O$  Near  $4.5 \mu$ ", J.Q.S.R.T., 12, 873 (1972).
23. Young, L.D.G., "Relative Intensity Calculations for Nitrous Oxide", J.Q.S.R.T., 12, 307 (1972).
24. P. Bletzinger and C.A. DeJoseph Jr., "Effect of Oxygen and Hydrogen on Electron Beam Discharges in Atmospheric Pressure  $CO_2$  Mixtures", paper H-2 at Gaseous Electronics Conference, Pittsburgh (1979).
25. Deutsch, T.F., "Effect of Hydrogen on  $CO_2$  TEA Lasers", Appl. Phys. Lett., 20, 315 (1972).

## Appendices

## APPENDIX I

Description of the Fourier Transform Spectrometer Calibration program FTICAL. This program is a modified version of a program appearing in Tables of Wave numbers for the Calibration of Infrared Spectrometers compiled by A.R.H. Cole, 2nd edition, Pergamon Press, 1977, pp. 202-205.

The program fits a set of up to 100 standard lines to one of two fitting functions. In normal usage, the standard lines are fit to the function,

$$\sigma(\text{standard}) = \sigma_1 \cdot \frac{n(\text{HeNe})}{n(\sigma_1)} \quad (\text{A-1})$$

where,

$$\sigma_1 = \frac{\sigma(\text{measured})}{1-a} \quad (\text{A-2})$$

and the parameter 'a' is determined by the method of least-squares.  $n(\text{HeNe})$  and  $n(\sigma_1)$  are the indices of refraction of air at the wavenumber of the helium-neon laser and wavenumber  $\sigma_1$ . The program may also be used to fit the standard lines to a non-linear function of the form,

$$\sigma_1 = a_1 + a_2\sigma + a_3\sigma^2 + a_4\sigma^3 \quad (\text{A-3})$$

where  $\sigma$  is the measured line position and the  $a_i$ 's are determined by least-squares. The fitting function used is determined by the user by setting the parameter SWITCH to either 1 or 0. After the fitting functions is determined, measured line positions of unknown lines are read-in and corrected according to either equation (A-2) or (A-3) and equation (A-1). For extrapolation out of the wavenumber region of the standard lines, equation (A-3) (SWITCH = 0) should not be used. For interpolation within the wavenumber region on the standard lines, either equation (A-2) or (A-3) may be used.

Description of the input parameters:

PR - Sets the maximum allowable error (in  $\text{cm}^{-1}$ ) between the corrected measurements and the known values of the standard lines used. After a least-squares fit is made to the known standards, the maximum error is found between the corrected measurements and the known line positions of the standards. If this maximum error exceeds the value PR, the measurement that yielded this error is removed from the set of measured values and the least-squares fit is repeated. This rejection process continues until the maximum error no longer exceeds PR. If PR = 0, all measured values are used.

SWITCH - This parameter determines which fitting function is chosen. If SWITCH = 1, equation (A-2), which is linear in the measured values, is used. If SWITCH = 0, equation (A-3), which is non-linear in the measured values, is used.

TEMPC and PRESC - The air temperature (deg. C) and barometric pressure (mm of Hg) at which the standard lines were measured.

TEMPU and PRESU - The air temperature (deg. C) and barometric pressure (mm of Hg) at which the standard lines were measured.

Some additional notes to the user of FTCAL are in order. All cards read by FTCAL except the first card, are read in the list directed read format of the CDC6600. Data may be placed anywhere on a card and if more than one parameter is to be read from a card, the parameters may be separated by spaces, commas, or other symbols (see CDC6600 manual). The first number on a standard line card and an unknown line card are for line identification. For standard lines this can be an integer from 0 to 999; for unknown lines this can be an integer from 0 to 9999. If the number of standard lines used is less than that needed for a least-squares fit to the fitting function chosen (SWITCH = 0), the function is truncated starting with the highest powers of the measured values.

A listing of FTAL is given on the following pages. The comment cards explain the order that the data should appear on cards.

```

1  PROGRAM FICAL(INPUT,OUTPUT)
2  CALIBRATION PROGRAM FOR FOURIER TRANSFORM SPECTROMETER
3  FIRST CARD-COLS 1-30 FOR A TITLE
4  SECOND CARD-PR (REJECTION CRIT. RIA)
5  THIRD CARD-SWITCH (1=LINEAR FIT, 0=CUBIC FIT)
6  FOURTH CARD IS FOR TEMP.(DEG C) AND BAROMETRIC PRESSURE(MM HG)
7  AT WHICH THE STANDARD LINES WERE MEASURED
8  STANDARD LINES FOLLOW-MAXIMUM NUMBER IS 10
9  FIRST NUMBER ON THE CARD IS FOR LINE IDENTIFICATION
10 SECOND NUMBER IS FOR THE LINE POSITION MEASUREMENT
11 THIRD NUMBER IS FOR WAVELENGTH OF STANDARD LINE
12 THE LAST CARD WITH A KNOWN WAVELENGTH TO 9. USID FOR
13 CALIBRATION MUST BE FOLLOWED BY A CARD WITH THREE ZEROS
14 PUNCHED WITH SPACES BETWEEN ZEPHS
15 NEXT CARD IS FOR TEMP. AND PRES DATA FOR UNKNOWN
16 UNKNOWN LINES FOLLOW-SAME FORMAT AS STANDARD LINES BUT WITHOUT
17 WAVELENGTH
18 MORE THAN ONE BATCH OF STANDARDS AND UNKNOWN CAN BE RUN IN
19 SUCCESSION IF A CARD WITH -1 IS PLACED BETWEEN BATCHES
20 THE LAST CARD IN THE DECK MUST BE THREE ZEROS AS ABOVE
21
22 READ AND WRITE STATEMENTS ARE FOR COCOS60 ONLY
23
24 DOUBLE PRECISION JX,VJ,VJ,TEMP,HENX,C,A,D,P,R,C,C,ON,C1
25 DIMENSION C(10),A(4,5),C(10,10),TITLE(12)
26
27 FUNCTION JX IS THE INDEX OF REFRACTION OF THE AIR MANS ONE
28
29 JX=((J,T,P))=(0.0003280-35+2.9-351000/(1.0010-V*V)+2.550000/(L-1.009
30 6-V*V))*1.004500/(1.000+3.650-63*TE)*PE/7.6002
31
32 10 READ(10,1),TITLE(1),I=1,12
33 1000 FORMAT(12A5)
34 READ*,PR
35 READ*,SWITCH
36 READ*,TEMP,PR,SC
37 LET=4PC
38 PE=PRESSC
39 HENX=DEX(1.6748014,TEMP)+1.000
40 SWITCH=SWITCH
41
42
43 READ STANDARD LINES ONE AT A TIME AND SET UP ARRAY FOR LEAST
44 SQUARES TREATMENT
45
46 20 READ*,D(1),A1,M1
47 IF(A1-1.0,3.0)GO TO 35
48 N=4
49 C1=A1
50 C(1,1)=1.000
51 C(1,2)=C1
52 C(1,3)=C1*C1
53 C(1,4)=C1*C1*C1
54
55 THE NEXT TWO STATEMENTS CORRECT FOR THE DISPERSION OF THE INDEX
56 OF REFRACTION OF THE AIR BETWEEN THE STANDARDS AND THE MEAN-CLASS
57
58 WNU=41

```



```

115 160 CONTINUE
120 3
      REJECTION ROUTINE
170 IF (PR)230,290,180
180 X=).
      DO 230 J=1,N
      IF (C(J,3))190,230,230
190 Y=C(J,3)
      GO TO 210
200 Y=C(J,3)
210 IF (V-X)230,230,220
220 NH=J
      X=Y
230 CONTINUE
240 IF (P2-X)240,250,290
240 DO 250 J=1,1
      D(J)=C(NH,J)
250 C(NH,J)=0.
      NH=NH+1
      DO 260 M=1,1
      DO 260 J=NH,N
260 C(J-1,J)=C(J,J)
      DO 270 J=1,1
270 C(J,J)=0(J)
      GO BACK AND DO LAST SQUARES
140 3
      NH=1
      DO 10 TO -0
290 PRINT(40, (TITLE(I),I=1,12)
1040 FORMAT(1H,12A5)
      PRINT(5,N,PR
1050 FORMAT(1HJ,17HNO. OF STD LINES=13,17H REJECTION LIMIT=F5.3)
      PRINT(2,TEMPC
      PRINT(3,PR,SC
1052 FORMAT(1H,35TEMPERATURE DURING CALIBRATION RUN=F5.1,6H DEG.C)
1053 FORMAT(1H,24BAROMETRIC PRESSURE=F8.1,7H MM HG.)
      IF (ISHIGH,230)GO TO 235
      PRINT(55
1055 FORMAT(1HJ,4HLINEAR CORRECTION IN EFFECT-CONSTANT IS)
      PRINT(70,A(2,4M1)
      GO TO 285
285 PRINT(58
1050 FORMAT(1HJ,22HCONSTANTS OF CUBIC EDN)
      PRINT(70,(A(J,141),J=1,44)
1070 FORMAT(1H,5X,17.10)
285 PRINT(33
1080 FORMAT(1HJ,6.4 NO. MEAS DIFF)
      NH=NH+1
      DO 300 J=1,NH
      IN1=C(J,6)
      A2=C(J,7)
      W1=C(J,13)
      W2=C(J,9)
      DIF=C(J,3)
      IF (J,31,NH)GO TO 290

```



```

1100 PRINT13,IN1,A2,M1,M2,JIF
1101 FORMAT(1H ,13,9X,F9.3,12X,F10.4,12X,F9.3,9X,F7.3)
1102 GO TO 300
1103 PRINT12,IN1,A2,M1,M2,JIF
1104 FORMAT(1H ,13,9X,F9.3,12X,F10.4,12X,F9.3,9X,F7.3,1H*)
1105 CONTINUE
1106 IF(N-NUM)510,320,320
1107 PRINT11,3
1108 FORMAT(1H ,13H*REJECTED LINE)
1109 PRINT11,0
1110 PRINT11,0
1111 FORMAT(1H,8H RESULTS)
1112 READ*,TEMPU,PRESU
1113 J=TEMPU
1114 PRESU
1115 PRINT11,3,TEMPU
1116 PRINT11,3,PRESU
1117 FORMAT(1H,31H TEMPERATURE DURING UNKNOWN RUNS,F9.1,6H 950.C)
1118 HEXEX=DEX(1.573800E-7E,P,1)+1.00
1119 PRINT11,3
1120 FORMAT(1H,6H NO.
1121 6H WAVE)
1122 READ A LINE TO 1. CALIBRATED
1123 READ*,DN1,A2
1124 IN1=DN1
1125 IF(1H,17.0)GO TO 10
1126 IF(A2.0201.0)STOP
1127 C2=A2
1128 THE NEXT TWO STATEMENTS ARE THE LEAST-SQUARES ADJUSTMENT AND THE
1129 DISPERSION CORRECTION
1130 UN1=A(1,141)+C2*(A(2,141)+C2*(A(3,141)+C2*(A(4,141)))
1131 A2=V1J*HEALX/DEX(VAD,TE,P,1)+1.00
1132 PRINT11,3,IN1,A2,M2
1133 FORMAT(1H ,14,9X,F9.3,12X,F9.3,1H*)
1134 GO TO 330
1135 END

```

## APPENDIX II

On the following pages is a listing of the program CODIAG and its associated subroutines and function subprograms. The programs are well commented so little explanation will be given here. One important point is worth mentioning. The parameter NDP (fourth card, first number) determines the assumed resolution of the interferometer. It should reflect any effects due to finite source size and should only include data points on one side of the interferogram.

## PROGRAM CODING(INPUT,OUTPUT,PLOT)

THIS IS THE MAIN DRIVING PROGRAM FOR DETERMINING THE ROTATIONAL TEMPERATURE AND THE VIBRATIONAL POPULATION DISTRIBUTION OF CARBON MONOXIDE BY OBSERVING THE INFRARED EMISSION FROM THE HOT GAS. THE PROGRAM CAN BE USED WITH EMISSION SPECTRA FROM EITHER THE FUNDAMENTAL, FIRST OVERTONE, OR SECOND OVERTONE. INTENSITIES CAN BE EITHER ABSOLUTE (WATTS/STERADIAN/CM<sup>2</sup>/CM) OR RELATIVE. THE PROGRAM ASSUMES THAT THE INSTRUMENT RESOLUTION IS MUCH GREATER THAN THE WIDTH OF THE LINES, AND ASSUMES INSTRUMENT FUNCTIONS OF THE KIND EXPECTED FROM AN INTERFEROMETER.

## SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED

SUBROUTINE ROTEM(TEMP,END,TEMP)  
CALCULATES THE ROTATIONAL TEMPERATURE OF THE GAS  
SUBROUTINE VIBDIS(TEMP,XMEAS,YMEAS,NPV,VNCL,INIV,YOFFSL,TEMP)  
CALCULATES THE VIBRATIONAL POPULATION DISTRIBUTION OF CO  
SUBROUTINE SPECANV(LEVEL,YOFFSL,TEMP,MIN,MAX,ROUT,YOUT,IN)  
CALCULATES A THEORETICAL EMISSION SPECTRUM USING THE  
VIBRATIONAL DISTRIBUTION AND ROTATIONAL TEMPERATURE CALCULATED  
SUBROUTINE PLOTOR(XIN,YIN,YNTRY,XDATA,YDATA,XFX,FY,  
AF,XFF,FY,FLY,FLY,IOPTN,LABEL)  
TAKES A PLOT OF THE THEORETICAL SPECTRUM CALCULATED IN SPECAN  
AND PLOTS THE MEASURED DATA ON THE SAME SET OF AXES

A NUMBER OF OTHER SUBROUTINES AND FUNCTION SUBPROGRAMS ARE CALLED BY THE ABOVE ROUTINES. THE USER OF THIS PROGRAM IS REFERRED TO THE COMMENTS IN THE ABOVE ROUTINES FOR A LIST OF THESE ADDITIONAL ROUTINES REQUIRED.

WITH THE EXCEPTION OF THE FIRST TWO DATA CARDS, ALL DATA IS READ IN THE LIST DIRECTED READ FORMAT OF THE C00000. IN THIS FORMAT, DATA MAY APPEAR ANYWHERE ON A CARD AND MAY BE SEPARATED BY BLANK SPACES, COMMAS, ETC. THE USER IS REFERRED TO THE C00000 FORTRAN EXTENDED REFERENCE MANUAL FOR A COMPLETE DESCRIPTION OF THIS FORMAT.

## DATA CARDS

FIRST CARD - COLUMNS 1-60 FOR A TITLE  
SECOND CARD - COLUMNS 1-20 FOR DATE AND RUN NUMBER  
THIRD CARD - 1ST NUMBER IS DATA V FOR THE DATA BEING USED.  
2ND NUMBER IS TO INDICATE IF INTENSITIES ARE  
ABSOLUTE - 0=RELATIVE INTENSITIES, 1=ABSOLUTE  
FOURTH CARD - CONTAINS FOUR PARAMETERS ASSOCIATED WITH THE  
INTERFEROMETER AND PERTAINING TO THE DATA COLLECTION. THEY ARE AS FOLLOWS  
1ST NUMBER-NUMBER OF DATA POINTS TAKEN  
2ND NUMBER-NUMBER OF TRANSFORM POINTS  
3RD NUMBER-HOLLERITH CHARACTERS DESCRIBING THE  
APODIZATION FUNCTION USED IN THE TRANSFORM.  
ONE OF THREE CAN BE USED  
0X-BOXCAR APODIZATION  
TI-TRIANGULAR APODIZATION  
AG-HAPP GENZEL APODIZATION  
(IN THE LIST DIRECTED READ FORMAT, FULL PATH  
CHARACTERS MUST BE IN QUOTES, SUCH AS "HG")  
4TH NUMBER-THE SAMPLE SPACING OF THE DATA POINTS

FIFTH CARD - PRINTOUT CONTROL FOR ROTEM, USED PRINTOUT  
 1=DATA FROM ROTEM IS PRINTED OUT  
 SIXTH THRU NTH CARD- DATA FOR USE IN ROTATIONAL TEMPERATURE  
 DETERMINATION. 1ST NUMBER ON CARD SIX IS THE NUMBER  
 OF DATA POINTS TO BE READ (UP TO 50). THE DATA  
 POINTS FOLLOW: X(1),Y(1),X(2),Y(2),... AFTER THE  
 LAST DATA POINT, THE ESTIMATED STANDARD DEVIATION  
 OF THE INTENSITIES SHOULD BE PUNCHED.  
 SEVENTH CARD - PRINT CONTROL FOR VIBDIS, EITHER 0,1,2, OR 3  
 0=NO PRINTOUT FROM VIBDIS

1=PRINTOUT OF POPULATION DISTRIBUTION AND LINE-  
 PRINTER PLOT OF OCCUPATION NUMBERS  
 2=STATISTICS FROM REGRES AND CALCULATED COEF.  
 3=OPTIONS 1 PLUS 2

NEXT CARD THRU M CARDS- DATA FOR VIBDIS. JUST AS IN ROTEM, 1ST  
 NUMBER IS THE NUMBER OF DATA POINTS (UP TO 100),  
 THEN THE DATA POINTS, THEN THE STANDARD DEVIATION.  
 NEXT CARD - 1ST NUMBER IS THE HIGHEST VIBRATIONAL LEVEL TO BE  
 INCLUDED IN THE ANALYSIS (UP TO V=33). 2ND NUMBER  
 IS THE CO PARTIAL PRESSURE (TORR).

NEXT CARD - PLOT OPTION. 0=NO PLOT, 1=CALCOMP PLOT OF  
 THEORETICAL SPECTRUM AND MEASURED DATA.

NEXT CARD(OPTIONAL)- IF A CALCOMP PLOT HAS BEEN REQUESTED, THIS  
 CARD CONTAINS A NUMBER WHICH DESCRIBES VARIOUS PLOT  
 OPTIONS. EITHER 0,1,2, OR 3

0-NORMAL PLOT SEQUENCE. THEORETICAL SPECTRUM AND  
 MEASURED DATA ARE PLOTTED AND THE USER MUST  
 SPECIFY THE LIMITS ON THE X-AXIS AND Y-AXIS  
 1-AS ABOVE EXCEPT NO MEASURED DATA IS PLOTTED  
 2-AS 1,0 EXCEPT THE USER NEED ONLY SPECIFY THE  
 LIMITS ON THE X-AXIS. THE Y-AXIS IS SCALED TO 8  
 INCHES.

3-AS IN 2 EXCEPT NO DATA IS PLOTTED

NEXT CARD(OPTIONAL)- IF A CALCOMP PLOT IS DESIRED, THIS CARD IS  
 FOR SPECIFYING THE PLOT LIMITS ON THE X AND Y AXIS.

1ST NUMBER-STARTING WAVELENGTH FOR THE X-AXIS

2ND NUMBER-LAST WAVELENGTH FOR THE X-AXIS

3RD NUMBER-CHANGE IN WAVELENGTH PER INCH

4TH NUMBER-THE INTENSITY MINIMUM FOR THE Y-AXIS

5TH NUMBER-THE INTENSITY MAXIMUM FOR THE Y-AXIS

6TH NUMBER-CHANGE IN INTENSITY PER INCH  
 (THE LAST THREE NUMBERS CAN BE ZERO IF PLOT OPTION  
 2 OR 3 ARE CHOSEN)

VERSION 02-20-73-1 FEB. 23, 1976 G. BRUNSLPH, JR.

COMMON/Z/NUP,SSP,IAFN,NTP,IGELTAV,IFAB

COMMON/W/4E,MEXE,AY,4,ZE,MEAS,ME3E,BE,ME,GE,J,DOE,JOS,PE,PH,LINE

COMMON/SCALIT/NX,NY,NXT,NTY,LINPIN,IGRID

COMMON/FF/XTHRY(2000),YTHRY(2000)

J1=J1=J1 TITLE(6),LOAT(12),XMEAS(100),YMEAS(100),XNU4V(40)

DATA 4E,MEXE,AY,MEZE,MEAL,ME3E/2169.0135002,13.2383076,1.051127E

6-2,0.744E-5,9.931E-7,3.1600E-8/

DATA 3,AL,GE,DE,DOE,83E,PE,ME,SE/1.93128,072,1.750,121E-2,9.43

67E-7,-2.541E-8,0.121403E-6,1.126E-9,1.0051E-10,0.5272E-12,1.737E

6-13/

READ TITLE AND DATE

```

115      READ(J3,(TITLE(I),I=1,6)
100      FORMAT(6A10)
120      READ(J3,LODATE(1),LODATE(2)
120      FORMAT(2A10)

120      READ DELTA V AND ABSOLUTE INTENSITY FLAG

125      READ*,DELTA V,FFA3
100      IODELTAV=IFIX(ODELTAV)
100      IFAB=IFIX(FFA3)

130      READ INTERFEROMETER DATA

135      READ*,FNOP,FNTP,IAFN,SSP
100      NOP=IFIX(FNOP)
100      NTP=IFIX(FNTP)

135      READ ROTATE PRINT CONTROL

135      READ*,PRINT1
100      IPRINT1=IFIX(PRINT1)
100      IF(IPRINT1.EQ.0)GO TO 140
130      PRINT139,(TITLE(I),I=1,6)
130      FORMAT(6H1,1X,6A10)
135      PRINT139,LODATE(1),LODATE(2)
135      FORMAT(6H1,1X,2A10)
137      PRINT137,NOP,NTP,IAFN,SSP
137      FORMAT(6H1,1X,INTERFEROMETER PARAMETERS: NOP=*,1X,NTP=*,1X,IAFN=*,1X,SSP=*,1X,FFA3=*,1X)
135      IF(IODELTAV.EQ.0)PRINT139,IODELTAV
135      IF(IAFN.EQ.0)PRINT139,IODELTAV
135      FORMAT(6H1,1X,DELTA V FOR THIS DATA=*,1X,IAFN,*,1X,SSP=*,1X,FFA3=*,1X)
135      WRITE(WATTS/STICK/MAVENUMBER,*)
135      FORMAT(6H1,1X,DELTA V FOR THIS DATA=*,1X,IAFN,*,1X,SSP=*,1X,FFA3=*,1X)
135      WRITE(WATTS/STICK/MAVENUMBER,*)

140      GET THE ROTATIONAL TEMPERATURE

140      CALL ROTEM(IPRINT1,FFNO,TEMP)

140      READ VISDIS PRINT CONTROL

145      READ*,PRINT2
100      IPRINT2=IFIX(PRINT2)
100      IF(IPRINT2.EQ.0)IPRINT1,NL,0)GO TO 160
100      PRINT139,(TITLE(I),I=1,6)
100      PRINT139,LODATE(1),LODATE(2)
100      PRINT137,NOP,NTP,IAFN,SSP
100      IF(IAFN.EQ.0)PRINT139,IODELTAV
100      IF(IAFN.EQ.0)PRINT139,IODELTAV

150      GET THE VIBRATIONAL DISTRIBUTION

160      CALL VIBDIS(IPRINT2,XFEAS,YFEAS,NPV,XNUAV,IHIV,CUFFSET,TEMP)

170      CHECK FOR A CALCUMP PLOT

```

```

175      READ*,FPL0T
          IPLOT=IFIX(FPL0T)
          IF (IPLOT.EQ.0) GO TO 1000
180      YOU WANTED A PLOT, SO WHICH TYPE?
          READ*,OPTION
          IOPTN=IFIX(OPTION)
          HOW BIG?
185      READ*,FXF,FLXF,CAF,FVE,FLY,CYE
          CHECK TO SEE IF WAVELENGTHS ARE INCREASING
          IF (FXF.LT.FLXF) GO TO 170
          XMIN=FLXF
          XMAX=FXF
          GO TO 180
190      XMIN=FXF
          XMAX=FLXF
          GENERATE THEORETICAL SPECTRUM
195      CALL SPECN(XNUMV,IMIV,YOFFSET,TEMP,XMIN,XMAX,XTHRY,YTH_LRY,NTHRY)
          NOW THAT YOU'VE GOT IT....PLOT IT....
200      CALL PLOTOR(XTHRY,YTHRY,NTHRY,XMEAS,YMEAS,NPV,FXF,FLXF,CXF,FVE,
          bFLYE,CY,CIOPT,LDATE)
          STOP
          END

```

SUBROUTINE ROTEMPRNT,FMU,TEMP)

THIS SUBROUTINE CALCULATES THE ROTATIONAL TEMPERATURE OF HOT CARBON MONOXIDE BY COMPARING THEORETICAL INTENSITIES WITH MEASURED INTENSITIES OF THE ROTATION OF THE  $v=0$  TO  $v=1$  TRANSITION. THE PROGRAM USES THE METHOD OF LEAST-SQUARES TO DETERMINE THE NUMBER DENSITY IN THE  $v=0$  LEVEL AND THE ROTATIONAL TEMPERATURE OF THE CO.

DESCRIPTION OF PARAMETERS

IPRNT - DATA PRINTOUT CONTROL (INPUT)

+1 PROGRAM PRINTS OUT MEAS. AND CALC. VALUES

0 NO PRINTOUT

FMU - NUMBER DENSITY IN THE  $v=0$  LEVEL (OUTPUT)

TEMP - ROTATIONAL TEMPERATURE OF THE GAS (OUTPUT)

OTHER INPUT IS VIA READ STATEMENTS AND COMMENTS- THE DATA IS READ IN A LIST DIRECTED READ FORMAT IN PAIRS, IE. X(1),Y(1),X(2),Y(2) ... WHERE X IS THE MEASURED WAVELENGTH AND Y IS THE INTENSITY.

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED

CURFIT - DETERMINES LEAST SQUARES FIT

FIT - CALLED BY CURFIT (SEE CURFIT)

FORIV - CALLED BY CURFIT (SEE CURFIT)

MINIV - CALLED BY CURFIT (SEE CURFIT)

ESTIN - CALLED BY FIT

SPASS - CALLED BY FIT

F - CALLED BY ESTIN

COMMENTS

DEVIATION STATEMENT VALID FOR UP TO 50 DATA POINTS

WKSJ04 03-J1-70-1 MAR. 11, 1970 C. DEJOS-PIH, JR.

COMMON/Z/NP,SSP,IAFM,IP,DELTA,IFAB

COMMON/W/M,WCX,WCY,WCZ,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

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DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

DELTA,WCAL,WCBL,WCME,WCDE,WCLE,WCPE,WCNE,WCSE,WC

SET UP INITIAL GUESSES FOR CURFIT (INITIALIZE PRM ARRAY)

```

0*****THIS IS THE INITIAL GUESS AT ROTATIONAL TEMP_RATJRC*****
0
00 PRM(1)=500.0
0
0*****
0 PR1(2)=1.
0 PR1(2)=FMAX/F10(MAV,ISV,PRM)
0 PR1(3)=0.0
0
0 SET UP INCREMENTS OF PRM FOR DERIVATIVE CALCULATIONS
0
00 OP=PM(1)=1.0
00 OP2(2)=0.01*PRM(2)
00 OP2(3)=0.01*FMAX
0
0 GET CURFIT
0
00 CALL CURFIT(MAV,FINT,SOY,NPK,3,MODL,PRM,OPRM,SIGF,.001,YFNT,CHIA)
0
0 PREPARE FOR PRINTOUT OR RETURN
0
00 FMO=PR1(2)
00 TEMP=PRM(1)
00 IF(IPRNT.EQ.0)GO TO 100
00 PRINT150
00 150 FORMAT(1H0,8X,5H****DATA FROM ROTATIONAL TEMP_RATJRC DETERMINATIO
00 6N****)
00 IF(MODL.EQ.0)GO TO 12
00 PRINT100,MODL,SIGMA
00 160 FORMAT(1H0,1X,*MODL=*,12,/,2X,*STANDARD DEVIATION ASSUMED FOR THE
00 6MEASURED INTENSITIES=*,1P=10.3)
00 GO TO 15
00 12 PRINT170,MODE
00 170 FORMAT(1H0,1X,*MODE=*,12,5X,*(NO WEIGHTING)*)
00 180 PRINT200,TEMP,SIGP(1)
00 200 FORMAT(1H0,1X,*ROTATIONAL TEMPERATURE=*,1P=10.3,* D=0.K*/2X,*ESTI
00 6MATED STANDARD DEVIATION=*,1P=10.3,* D=0.K*)
00 PRINT300,IO,LTAV,FMO,SIGP(2)
00 300 FORMAT(1H0,1X,*NUMBER DENSITY IN THE V=*,12,* LEVEL=*,1P=10.3,* C4
00 6-3*/2X,*ESTIMATED STANDARD DEVIATION=*,1P=10.3,* C4-3*)
00 PRINT300,PRM(3),SIGP(3)
00 350 FORMAT(1H0,1X,*ZERO OFFSET OF INTENSITIES=*,1P=10.3,* +0K=*,1P=10.3)
00 PRINT+30
00 400 FORMAT(1H0,1X,*WAVENUMBER=*,0X,*MEAS. INTENSITY*,0X,*CALC. INTENSIT
00 6Y*,5X,*PERCENT DIFF.*)
00 JIFT=0.
00 20 J=1,NPK
00 JIF=(FINT(J)-YFNT(J))/FINT(J)*100.
00 JIFT=JIFT+ABS(JIF)
00 20 PRINT500,MAV(J),FINT(J),YFNT(J),JIF
00 500 FORMAT(1H ,1X,F6.2,10X,1P=10.3,10X,1P=10.3,1X,UPF6.1)
00 FMPR=NPR
00 JIFT=JIFT/FMPR
00 PRINT500,JIFT,CHIA
00 600 FORMAT(1H0,1X,*AVERAGE ABSOLUTE ERROR=*,F6.1,* P.R.ENT=*,/,2X,*CHI-
00 6SQUARE=*,1P=12.0)
00 RETURN

```



SUBROUTINE VIBULS(IPRNT,XMEAS,YMEAS,IPV,VNCL,IPV,OFFSET,TEMP)  
 THE PURPOSE OF THIS PROGRAM IS TO CALCULATE THE VIBRATIONAL  
 POPULATION DISTRIBUTION OF CARBON MONOXIDE UNDER DISCHARGE CONDIT-  
 IONS. THE CALCULATION IS DONE BY COMPARING MEASURED SPECTRA FROM  
 EITHER THE FUNDAMENTAL, FIRST OVERTONE, OR SECOND OVERTONE WITH  
 THEORETICAL SPECTRA. THE LEVEL POPULATIONS ARE DETERMINED BY THE  
 METHOD OF LEAST SQUARES USING A MULTIPLE LINEAR REGRESSION ROUTINE.

DESCRIPTION OF PARAMETERS

IPRNT - PRINTOUT CONTROL PARAMETER (INPUT)

0 - NO PRINTOUT

1 - A LINE-PRINTER PLOT OF THE RELATIVE OCCUPATION  
 NUMBERS AND THE CALCULATED NUMBER DENSITIES IS MADE

2 - A PRINTOUT OF THE CALCULATED COEFFICIENTS FROM  
 REGRES WITH STATISTICS IS MADE

3 - OPTION 1 + OPTION 2

XMEAS - THE ARRAY OF MEASURED WAVELENGTHS (OUTPUT)

YMEAS - THE ARRAY OF MEASURED INTENSITIES (OUTPUT)

IPV - THE NUMBER OF DATA POINTS USED IN THE FIT (OUTPUT)

VNCL - THE ARRAY OF CALCULATED LEVEL POPULATIONS (VNCL(I) IS

THE NUMBER OF MOLECULES IN THE I-1 JIB. LEVEL, OUTPUT)

IPV - THE HIGHEST VIBRATIONAL LEVEL INCLUDED IN THE FIT (THE

SIZE OF THE VNCL ARRAY IS IPV+1, OUTPUT)

OFFSET - CALCULATED OFFSET OF ZERO INTENSITY (OUTPUT)

TEMP - THE ROTATIONAL TEMPERATURE OF THE GAS (INPUT)

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED

REGRES - MULTIPLE LINEAR REGRESSION ROUTINE

PLPLOT - LINE-PRINTER PLOT ROUTINE

MATINV - SYMMETRIC MATRIX INVERTER, CALLED BY REGRES

FCF4 - INTERMEDIARY BETWEEN REGRES AND FNV, CALLED BY REGRES

FNV - CALCULATES INTENSITY CONTRIBUTIONS FROM DIFFERENT VIB.

LEVELS, CALLED BY FCF4

IPASS - CALCULATES INSTRUMENT FUNCTION, CALLED BY FNV

STEIN - CALCULATES EINSTEIN A AND B COEFFICIENTS, CALLED BY FNV

F - CALCULATES HERMAN WALLACE FACTORS, CALLED BY STEIN

COMMENTS

ADDITIONAL INPUT IS THROUGH COMMONS AND READ STATEMENTS. XMEAS,  
 YMEAS, IPV, IPV, IPV ARE READ FROM CARDS AND SUPPLIED TO THE CALLING  
 ROUTINE THROUGH THE CALL LIST. IPRNT AND TEMP MUST BE SUPPLIED  
 BY THE CALLING ROUTINE. VNCL IS CALCULATED IN VIBULS AND IS  
 RETURNED TO THE CALLING ROUTINE THROUGH THE CALL LIST. DIMENSION  
 STATEMENTS VALID FOR IPV UP TO 100 AND IPV UP TO 39  
 VERSION 12-10-77 (SPECIAL WEIGHING) F-3,24,1977 COLUMBIA, JK.

COMMON Z/IDP,ISP,IAFN,NIP,IDECLAV,IFAB

COMMON W/MEM-XE,MEYCL,MZC,MEAL,MEJCL,AL,ALCL,ALCL,ALCL,ALCL,ALCL

COMMON SCALAT/NX,NY,NXT,NYT,LINPIN,TORLO

DIMENSION XMEAS(1),YMEAS(1),VNCL(1)

DIMENSION SIGM(100),YF(100),SIGMAV(40),RR(40),REL(40),RELJC(40),

EXXV(40)

W(1)=W\*(W+XE+V\*(WLYC+V\*(-WEZC+V\*(WALC-V\*WALC))))

WZEL=+ 50002

READ THE NUMBER OF DATA POINTS, THEN THE POINTS, THEN THE STANDARD

AD-A105 496

UNIVERSAL ENERGY SYSTEMS INC DAYTON OH

F/G 7/4

INVESTIGATION OF PLASMA EXCITATION. VOLUME III. ADVANCED OPTICA--ETC(U)

AUG 81 C A DEJOSEPH

F33615-77-C-3113

UNCLASSIFIED

707-3-F

AFWAL-TR-81-2082-VOL-3

NL

2 OF 2

AD A

105496


END

DATE

FILED

11-81

DTIC

DEVIAION OF THE MEASURED INTENSITIES. IF THE STANDARD DEVIATION  
IS SET TO ZERO, THE FIT IS NOT WEIGHTED

READ\*,NPV,(XMEAS(I),YMEAS(I),I=1,NPV),SIGG  
MODE=1  
IF(SIGG...0.0,J.)MODE=0

SET UP SIGN ARRAY

WEIGHTING FUNCTION IS ROUGHLY 1/INSTRUMENT FUNCTION

DO 20 I=1,NPV  
KFF=-0.24057+XMEAS(I)\*(1.23125+XMEAS(I)\*(-0.00051+XMEAS(I)\*(1.2  
6150E-2-XMEAS(I)\*9.0+58.7)))  
20 SIG(I)=0.23080/NFF\*SIGG

READ IM- HIGHEST LEVEL INCLUDED IN THE FIT, AND THE CO PARTIAL  
PRESSURE (TORR)

READ\*,IMIV,COPRES

GET READY TO CALL REGRES

NTT=IMIV+1-IDELTAV  
CALL REGRES(XMEAS,YMEAS,SIGM,NPV,NTT,TEMP,MODE,YET,AU,VNICAL,SGAJ,S  
6191AV,KK,RMUL,CHISQ,FTST)  
VOFF=JTEW

SINCE VNICAL CONTAINS NUMBERS FROM VEDELTA V TO V=I+IV, LOWER V'S  
MUST BE CALCULATED AND STORED IN VNICAL

DO 30 J=1,NTT  
K=NTT+IDELTAV-J+1  
30 VNICAL(K)=VNICAL(K-IDELTAV)

ASSUME THE LOWER LEVELS FOLLOW A THERMUR DISTRIBUTION

V1=ELJ0AT(IDELTAV)+.5  
V2=V1+1.  
JJ=IDELTAV+1  
A12=(5(V2)-5(V1))\*HCK/TEMP  
AKK=ALOG(VNICAL(JJ+1)/VNICAL(JJ))+A12  
DO 40 J=1,IDELTAV  
V3=ELJ0AT(J-1)+.5  
A13=(5(V1)-5(V3))\*HCK/TEMP  
40 VNICAL(J)=VNICAL(JJ)\*EXP(-FLOAT(JJ-J)\*AKK+A13)

NOW SET UP OCCUPATION NUMBERS

TOT=0.  
IM=IMIV+1  
DO 50 J=1,IM  
50 TOT=TOT+VNICAL(J)  
DENS=2.6172E19+273./TEMP+COPRES/760.

```

115      DO 50 J=1,NH
120      RELOC(J)=VNCAL(J)/TOT
        50 RELOC(J)=RELOC(J)*DENS
      00
      00 PREPARE FOR PRINTOUT OR RETURN
      00
      00 IF(IPRINT.EQ.0)GO TO 3000
      00 IF(IPRINT.EQ.1)GO TO 1000
      00 PRINT500
      000 FORMAT(1H0,7X,20H***DATA FROM VIBRATIONAL DISTRIBUTION DETERMINAT
        010H****)
      00 IF(MOD(-4,3)GO TO 70
      00 PRINT555,NPV,SIGG
      005 FORMAT(1H0,1X,*NUMBER OF DATA POINTS=*,15,2X,*STANDARD DEVIATION
        6 ASSUMED FOR THE MEASURED INTENSITIES=*,1P10.3)
      00 TO 30
      00 PRINT510,NPV
      010 FORMAT(1H0,1X,*NUMBER OF DATA POINTS=*,15,2X,*NO MEASUREMENTS*)
      00 PRINT525
      025 FORMAT(1H0,1X,*WAVELENGTH*,5X,*MEAN INTENSITY*,5X,*CALC. INTENSIT
        0Y*,2X,*PERCENT DIFF.**)
      00 DIFT=0.
      00 110 I=1,NPV
      00 IF(YMEAS(I)-YFT(I))/YMEAS(I)*100.
      00 JIFT=JIFT+ABS(DIF)
      010 PRINT530,XMEAS(I),YMEAS(I),YFT(I),JIF
      030 FORMAT(1H ,1X,F8.2,10X,1P10.3,10X,1P10.3,11X,2P10.1)
      00 NPV=NPV
      00 JIFT=DIFT/NPV
      00 PRINT535,JIFT,CHISQ
      035 FORMAT(1H0,1X,*AVERAGE ABSOLUTE ERROR=*,F8.1,* PERCENT*,/2X,*CHI-
        65 SQUARE=*,1P12.5)
      00 PRINT540,THIV,TEMP
      040 FORMAT(1H0,1X,*HIGHEST VIBRATIONAL LEVEL INCLUDED IN FIT=*,15,2X
        0,*ASSUMED ROTATIONAL TEMPERATURE=*,1P10.3,* 0.0.K*)
      00 PRINT550
      050 FORMAT(1H0,15X,32H***COEFFICIENTS FROM REGRES*****)
      00 PRINT560,A0,SGA0
      060 FORMAT(1H0,1X,*ZERO OFFSET OF INTENSITIES=*,1P-10.3,* +OR=*,10.3)
      070 PRINT570
      070 FORMAT(1H0,1X,*UPPER V*,5X,*CO-F.*5X,*-ST. STJ. DEV.*5X,*LINEAR
        0 CORRELATION COEF.**)
      00 120 A=1,NIT
      00 J=1,DELTAIV
      00 K=J-1
      120 PRINT580,K,VNCAL(J),SIGMAV(I),RR(I)
      000 FORMAT(1H ,2X,12,2X,1P10.3,5X,10.3,10X,11J.3)
      00 PRINT590,PMUL,FI,ST
      090 FORMAT(1H0,1X,*MULTIPLE LINEAR CORRELATION COEF.=*,1P-10.3,2X,*V
        0ALUE OF FI-ST=*,10.3)
      00 IF(IPRINT.EQ.2)GO TO 3000
      1300 PRINT700
      070 FORMAT(1H0,1X,*VIBRATIONAL POPULATION DATA--IF INTENSITIES ARE AND
        60LUTE, LAST COLUMN IS ABSOLUTE*)
      00 PRINT710
      0710 FORMAT(1H0,1X,*VIB. LEVEL*,3X,*REL. OCCUPATION NO.*5X,*REL. NO. J
        0 BENSITY*,5X,*NO. IN LEVEL*)

```

```
175 YMIN=YMAX=RELOC(I)
    DO 130 I=1,IM
      L=I-1
      PRINT720,L,RELOC(I),XELN(I),VNCAL(I)
      720 FORMAT(IH,5X,I2,12X,1PL10.3,12X,-10.3,10X,210.3)
      XXV(I)=L
      YMIN=AMIN1(YMIN,RELOC(I))
      130 YMAX=AMAX1(YMAX,RELOC(I))
      XMIN=L
      XMAX=FLOAT(IM-1)
      MD=12
      CALL PLOTIT(XXV,RELOC,IM,IM*,XMIN,XMAX,YMIN,YMAX,MMD,2)
      3J00 NEXT I
    END
```

185

```

SUBROUTINE SP_CON(XNV,L_VLL,YOFFSET,TMP,MIN,MAX,WOUT,YOUT,NN)
C
C THE PURPOSE OF THIS PROGRAM IS TO GENERATE A THEORETICAL EMISSION
C SPECTRUM FROM CARBON MONOXIDE. THE PROGRAM IS NORMALLY USED IN
C CONJUNCTION WITH THE AFAPL/POJ FOURIER TRANSFORM SPECTROMETER.
C THEREFORE SUCH QUANTITIES AS INSTRUMENT RESOLUTION, DATA POINT
C SPACING, ETC. ARE MATCHED TO THOSE OF THE INSTRUMENT BY THE COMMON
C /Z/. THE OUTPUT IS TWO ARRAYS WOUT AND YOUT WHICH ARE THE WAVE-
C NUMBERS AND INTENSITIES OF THE CALCULATED SPECTRUM.

```

```

C
C DESCRIPTION OF PARAMETERS

```

```

XNV - THE ARRAY OF NUMBER DENSITIES FOR THE VARIOUS
VIBRATIONAL LEVELS OF CO (GROUND STATE=XNV(1))
LEVEL - THE NUMBER OF THE HIGHEST LEVEL SUPPLIED BY XNV. (IF
L_VLL=J, THE ARRAY SIZE FOR XNV=J+1)
YOFFSET- CONSTANT ADDED TO EACH INTENSITY CALCULATED
TMP - THE ROTATIONAL TEMPERATURE OF THE GAS
MIN - THE LOWEST WAVELENGTH DESIRED FOR THE CALCULATION
MAX - THE HIGHEST WAVELENGTH DESIRED FOR THE CALCULATION
WOUT - THE ARRAY OF OUTPUT WAVELENGTHS
YOUT - THE ARRAY OF OUTPUT INTENSITIES
NN - THE NUMBER OF DATA POINTS GENERATED

```

```

C
C SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED

```

```

FNU(X,J,TEMP)

```

```

C
C CALCULATES THE INTENSITY CONTRIBUTION FROM VARIOUS VIB. LEVELS

```

```

C
C COMMENTS

```

```

WOUT AND MAX ARE LIMITS ON THE DATA. THE SPACING OF THE WOUT
ARRAY IS DETERMINED BY COMMON/Z/ SO THAT WOUT MIGHT NOT CONTAIN
WOUT AND/OR MAX.

```

```

VERSION 03-10-70-2

```

```

MAR. 13, 1976

```

```

G. C. JOSEPH, JR.

```

```

COMMON /Z/ NIP, SSP, IAFN, NTF, IDeltaTAV, IFAB

```

```

COMMON W/WE, WEX, WEY, WEZ, WEAL, WESE, SE, AE, GE, DE, JDE, JDEL, P, H, L, INC

```

```

DIMENSION WOUT(1), YOUT(1), XNV(1)

```

```

DIMENSION WVC(40)

```

```

C(1)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))

```

```

C(2)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(3)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(4)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(5)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(6)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(7)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(8)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(9)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(10)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(11)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(12)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(13)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(14)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(15)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(16)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(17)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(18)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(19)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(20)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(21)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(22)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(23)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(24)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(25)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(26)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(27)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(28)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(29)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(30)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(31)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(32)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(33)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(34)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(35)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(36)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(37)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(38)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(39)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))
C(40)=V*(W+V*(-WESE+V*(WEY-WEV*(-WEZ+V*(WEAL-WEV*WESE))))

```

```

C
C SET UP LIMITS ON WOUT ARRAY

```

```

FNU=NIP

```

```

IMIN=FIX(MIN*SSP*FNU/15790./2.)+1

```

```

IMAX=FIX(MAX*SSP*FNU/15790./2.)-1

```

```

NN=IMAX-IMIN+1

```

```

IF (NIP.GT.15790.) GO TO 200

```

```

JSTOP=L_VLL-IDeltaTAV+1

```

```

C
C LOCATE BAND CENTERS FOR EACH VIB. LEVEL

```

```

DO 10 J=1,JSTOP

```

```

WVC(J)=FNU*(J-1)+.5

```

```

WJP=VLC+FLOAT(IDeltaTAV)

```

```

10 WVC(J)=G(WJP)-G(VLC)

```

```

00000000  SET UP THE MOUT AND YOUT ARRAYS
00000000  NSLIDE=4
00000000  DO 70 I=1,NN
00000000  MOUT(I)=15796.*2./SSP/FNW*FLOAT(IMIN+I-1)
00000000  YOUT(I)=YOFFSET
00000000  DO 30 J=1,JSIUP
00000000  JVC=J
00000000  IF(MOUT(I).GT.MVC(J))GO TO 40
00000000  30 CONTINUE
00000000  40 IF(JVC=.4.)JSTOP=JVC=JSTOP+2
00000000  IF(JVC=.1,3)JVC=3
00000000  JWHIN=JVC+NSLIDE
00000000  JWHAX=JVC+NSLIDE
00000000  IF(JWHIN.LT.1)JWHIN=1
00000000  IF(JWHAX.GT.JSTOP)JWHAX=JSTOP
00000000  DO 50 J=JWHIN,JWHAX
00000000  WATCH JUT FOR THE DIFFERENCE IN INDEX DEFINITIONS BETWEEN FNW AND
00000000  XNV.
00000000  JJ=J+I*ELTAV
00000000  5- YOUT(I)=YOUT(I)+XNV(JJ)*FNW(MOUT,I,J,TEMP)
00000000  70 CONTINUE
00000000  THAT SHOULD DO IT.....
00000000  GO TO 1000
00000000  200 PRINT213
00000000  210 FORMAT(1H0,1X,*NUMBER OF POINTS REQUESTED ON PLOT -XC--US DIMENSIO
00000000  64 STATEMENTS---EXECUTION HALT_3*)
00000000  STOP
00000000  1000 RETURN
00000000  END

```

```

SUBROUTINE PLOTUX(XTHRY,YTHRY,NTHRY,XDATA,YDATA,FXF,FLXF,
  B,CXFX,FY,FYLY,IOPTN,LABEL)

```

```

C THE PURPOSE OF THIS PROGRAM IS TO PLOT BOTH THE THEORETICAL
  SPECTRUM AND THE MEASURED DATA POINTS FOR CARBON MONOXIDE EMISSION

```

```

C DESCRIPTION OF PARAMETERS

```

```

XTHRY - THE ARRAY OF WAVELENGTHS FOR THE THEORETICAL SPECTRUM
YTHRY - THE ARRAY OF INTENSITIES FOR THE THEORETICAL SPECTRUM
NTHRY - THE NUMBER OF POINTS TO BE PLOTTED IN THE THEOR. SPECT.
XDATA - THE ARRAY OF MEASURED WAVELENGTHS
YDATA - THE ARRAY OF MEASURED INTENSITIES
NDATA - THE NUMBER OF MEASURED DATA POINTS
FXF - THE FIRST WAVELENGTH ON THE PLOT AXIS
FLXF - THE LAST WAVELENGTH ON THE PLOT AXIS
CXFX - THE CHANGE IN WAVELENGTH FOR THE X-AXIS (WAVELENGTH/INCH)
FY - THE FIRST INTENSITY VALUE ON THE PLOT AXIS
FYLY - THE LAST INTENSITY VALUE ON THE PLOT AXIS
IOPTN - THE CHANGE IN INTENSITY FOR THE Y-AXIS (UNITS/INCH)

```

```

C CONTROLS PLOT OPTIONS
  0 - NORMAL PLOT SEQUENCE
  1 - NO DATA PLOTTED, ONLY THEORETICAL SPECTRUM
  2 - Y-AXIS IS SCALED TO 6 INCHES, FYLY, ETC. IGNORED
  3 - NO DATA IS PLOTTED, Y-AXIS SCALED TO 6 INCHES

```

```

C LABEL - TWO WORD ARRAY FOR PUTTING A CHARACTER TITLE ON PLOT

```

```

C COMMENTS

```

```

C THIS VERSION OF PLOTUX DESTROYS THE ARRAYS XTHRY AND YTHRY.
  IF IT IS DESIRED NOT TO DESTROY THESE ARRAYS, LEAVE THE C FROM
  COLUMN 1 OF THE FIRST DIMENSION STATEMENT AND REMOVE THE COMMON
  BLOCK /FF/.

```

```

C VERSION 02-20-75-1 Feb. 20, 1970 C. DEJUSEPH, JR.

```

```

COMMON /Z/ OP, SUP, IAF, NIP, IOLTA, IFAU

```

```

COMMON /FF/ XT(2000), YT(2000)

```

```

C DIMENSION XT(2000), YT(2000)

```

```

C DIMENSION XTHRY(1), YTHRY(1), XDATA(1), YDATA(1), LABEL(2)
  DATA YL/3.3/

```

```

C ESTABLISH THE ORIGIN AT X=0, Y=0

```

```

CALL PLOT(0,0,-1,0,-3)

```

```

CALL PLOT(0,0,0,0,-3)

```

```

NAX2=NIA-LY+2

```

```

NML=NTH-LY+1

```

```

IF(IOPTN-1) 3,3,10

```

```

C SCALE Y-AXIS

```

```

10 YMIN=YMAX=YTHRY(1)

```

```

DO 15 I=1,NTHRY

```

```

  Y1X=AMAX1(YMAX,YTHRY(I))

```

```

  Y1L=AMIN1(YMIN,YTHRY(I))

```

```

  IF(IOPTN-1) GO TO 20

```



```

60      DO 25 J=1,NDATA
          YMAX=A1AX1(YMAX,YDATA(I))
          YMIN=A1MIN(YMIN,YDATA(I))
          YP1=(YMAX+YMIN)/YL
          Y1(N2)=DYPLN
          Y1(N1)=YMIN
          GO TO 40
        25 YL=(FLY2-FY1)/CYL
          Y1N=FY1
          Y1(N2)=CYL
          Y1(N1)=FY1
          40 YMAX=Y 11+Y1(N2)*IFIX(YL)
          SCAL= X-AXIS
          XMIN=FXF
          XMAXG=FLXF
          IF(FXF.GT.FLXF)XMIN=FLXF
          IF(FXF.GT.FLXF)XMAXG=FXF
          XPIN=DXF
          XL=(FLXF-FXF)/CXF
          X1(N2)=DXPIN
          X1(N1)=FXF
          60      DRAW AXES
          CALL AXIS(0,0,11HMAVENUMBERS,-11,XL,0,X1(N11),X1(N2))
          IF(IFA3.NE.0)GO TO 45
          CALL AXIS(0,0,13HINTENSITY(RELATIVE),13,YL,0,Y1(N11),Y1(N2))
          GO TO 47
        45 CALL AXIS(0,0,32HINTENSITY(WATTS/STER/MAVENUMBER),32,YL,0,Y1(N11),Y1(N2))
          GO TO 47
        47      S-T J=1,NTHERY
          XT(J)=XTLERY(J)
          IF(XT(J).LT.XMIN)XT(J)=XMIN
          IF(XT(J).GT.XMAXG)XT(J)=XMAXG
          Y1(J)=YTHERY(J)
          IF(Y1(J).LT.YMIN)Y1(J)=YMIN
          50 IF(Y1(J).GT.YMAXG)Y1(J)=YMAXG
          CONNECT ARRAY POINTS
          CALL LINE(XT,Y1,NTHERY,1,5,0)
          PLOT MEASURED DATA?
          IF(IOPTN.EQ.1,04,IUPT4.EQ.3)GO TO 100
          N2=NDATA+2
          N1=NDATA+1
          X1(N2)=X1(N2)
          X1(N1)=X1(N1)
          Y1(N2)=Y1(N2)
          Y1(N1)=Y1(N1)
          DO 60 J=1,NDATA

```

```

115 AT(J)=XDATA(J)
    IF(XT(J).LT.XMIN)XT(J)=XMIN
    IF(XT(J).GT.XMAXG)XT(J)=XMAXG
    YT(J)=YDATA(J)
    IF(YT(J).LT.YMIN)YT(J)=YMIN
    IF(YT(J).GT.YMAXG)YT(J)=YMAXG
00   IF(YT(J).GT.YMAXG)YT(J)=YMAXG
      PLOT THE MEASURED DATA POINTS

      L=9
      CALL LINE(XT,YT,NDATA,L,-1,L)
      LABEL PLOT
00   00   00   00   00   00
      100 YTOP=YL+.5
          CALL SYMBOL(L6,YTOP,.245,LABEL(1),0.,10)
          CALL SYMBOL(.774,.798,.245,LABEL(2),0.,10)
          CALL PLOTE
            RETURN
              EN)

```





```

115 10+ HOUT=1
    GO TO 100
120 10+ HOUT=3
    IF HOUT=1
      IF (IT-25) 100, 103, 113
      GO 107 J=1, INTERM5
      A(J)=B(J)
      FLAMDA=FLAMDA/10.
      IF (FLAMDA.LT. J.JJ) FLAMDA=L. JUI
      IF (HOUT.EQ.0) GO TO 10
      GO 104 J=1, INTERM5
125 103 SIGMA4(J)=SQRT(ARRAY(J,J)/ALPHA(J,J))
      GO TO 115
130 103 PRINT1030, JSNG
      1030 FORMAT(* PARAMETER *, I2, * CHANGED SIGN---EXECUTION HALTED. *, /, * TX
      BY NEW INITIAL GUESSES. *)
      STOP
135 111 PRINT111.
      1110 FORMAT(* FLAMDA HAS BEEN INCREASED TEN TIMES, CHI SQUARE IS STILL *
      6, /, * INCREASING---EXECUTION HALTED. *)
      STOP
      113 PRINT1130
      1130 FORMAT(* 20 ITERATIONS COMPLETED, CONVERGENCE CRITERIA NOT MET--- *
      6EXECUTION HALTED*)
      GO TO 104
140 115 RETURN
      END

```

03/10/73 13:09:32

FIR 7.00000

SUBROUTINE MATINV 74/74 OPT=2

```

1  SUBROUTINE MATINV
2
3  PURPOSE
4  INVERT A SYMMETRIC MATRIX AND CALCULATE ITS DETERMINANT
5
6  USAGE
7  CALL MATINV(NORDER,DLT)
8
9  DESCRIPTION OF PARAMETERS
10  NORDER - DEGREE OF MATRIX (ORDER OF DETERMINANT)
11  DLT - DETERMINANT OF INPUT MATRIX
12
13  COMMENTS
14  DIMENSION STATEMENTS VALID FOR NORDER UP TO 40
15  THE ARRAY IS CARRIED THROUGH THE COMMON/AA/
16  VERSION 12-10-77-1 DEC. 13, 1977 G. J. JONES, PH. JK.
17
18  SUBROUTINE MATINV(NORDER,DLT)
19  DOUBLE PRECISION ARRAY,AMAX,SAVE
20  COMMON/AA/ARRAY(40,40)
21  DIMENSION IK(40),JK(40)
22  DET=1.
23  DO 100 K=1,NORDER
24  FIND LARGEST ELEMENT ARRAY(I,J) IN REST OF MATRIX
25
26  AMAX=0.0001
27  DO 30 J=K,NORDER-K
28  DO 30 J=K,NORDER-K
29  IF (ABS(AMAX)-ABS(ARRAY(I,J))) < 24,24,30
30  AMAX=ARRAY(I,J)
31  IK(K)=I
32  JK(K)=J
33  CONTINUE
34
35  INTERCHANGE ROWS AND COLUMNS TO PUT AMAX IN ARRAY(K,K)
36
37  IF (AMAX) *1,32,41
38  DET=0.0
39  GO TO 140
40  I=IK(K)
41  IF (I-K) 21,51,43
42  DO 50 J=I,NORDER
43  SAVE=ARRAY(K,J)
44  ARRAY(K,J)=ARRAY(I,J)
45  ARRAY(I,J)=SAVE
46  J=JK(K)
47  IF (J-K) 21,51,53
48  DO 60 I=1,NORDER
49  SAVE=ARRAY(I,K)
50  ARRAY(I,K)=ARRAY(I,J)
51  ARRAY(I,J)=SAVE
52  I=JK(K)
53  IF (I-K) 53,70,53
54  ARRAY(I,K)=ARRAY(I,J)
55  CONTINUE
56  DO 60 I=1,NORDER

```

SUBROUTINE MATINV

I=74 OPT=2

F16 10.9\*440

J1/10/79 10:19:32

P40-

2

```

50      DO 10 J=1,NORDER
       IF(I-K)74,50,74
       74 IF(J-K)75,80,75
       75 ARRAY(I,J)=ARRAY(I,J)+ARRAY(I,K)*ARRAY(K,J)
       80 CONTINUE
       DO 90 J=1,NORDER
       IF(J-K)93,90,93
       93 ARRAY(K,J)=ARRAY(K,J)/AMAX
       90 CONTINUE
       100 DET=DET*AMAX
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```

1  FUNCTION FCHISQ
2
3  PURPOSE
4  EVALUATE REDUCED CHI SQUARE FOR FIT TO DATA
5  FCHISQ=SUM((Y-YFIT)**2)/NFR--
6
7
8
9
10  J045-
11  RESULT=FCHISQ(Y,SIGMA,Y,NPTS,NFR,FREE,MODE,YFIT)
12
13  DESCRIPTION OF PARAMETERS
14  Y - ARRAY OF DATA POINTS
15  SIGMA - ARRAY OF STANDARD DEVIATIONS FOR DATA POINTS
16  NPTS - NUMBER OF DATA POINTS
17  NFR - NUMBER OF DEGREES OF FREEDOM
18  MODE - DELTA-METHOD OF WEIGHTING LEAST SQUARES FIT
19  +1 (INSTRUMENTAL) WEIGHT=1./SIGMA(I)**2
20  -1 (STATISTICAL) WEIGHT=1./Y(I)
21  0 (NO WEIGHTING) WEIGHT=1.
22  YFIT - ARRAY OF CALCULATED VALUES OF Y
23  VERSION 12-15-77-1 DEC. 15, 1977 G. J. JOSEPH, JR.
24
25  FUNCTION FCHISQ(Y,SIGMA,NPTS,NFR,FREE,MODE,YFIT)
26  DOUBLE PRECISION CHISQ,WEIGHT
27  DIMENSION Y(1),SIGMA(1),YFIT(1)
28  CHISQ=0.
29  IF (NFR) 13,13,20
30  GO TO 40
31
32  ACCUMULATE CHI SQUARE
33
34  DO 30 I=1,NPTS
35  IF (MODE) 22,27,29
36  IF (Y(I)) 25,27,23
37  WEIGHT=1./Y(I)
38  GO TO 30
39  WEIGHT=1./(-Y(I))
40  GO TO 30
41  WEIGHT=1.
42  GO TO 30
43  WEIGHT=1./SIGMA(I)/SIGMA(I)
44  CHISQ=CHISQ+WEIGHT*(Y(I)-YFIT(I))*(Y(I)-YFIT(I))
45
46  DIVIDE BY THE NUMBER OF DEGREES OF FREEDOM
47
48  FREE=NFR-1
49  FCHISQ=CHISQ/FREE
50  RETURN
51  END

```

SYMBOLIC REFERENCE MAP (M=1)







```

      KUTJ=2.*R4+1.
      CALL EST=IN(IGELTAV,IVLO,M,1,M,AA,JB)
      EX=X3(-HCKT*FVUP)
      FIL=AA*ROTJ*EX*BPASS(NUP,SSP,IAF4,XI,M)
      DERIV(2)=DERIV(2)+FIL
      DERIV(1)=DERIV(1)+FVUP*HCKT*A11+FIL
      Q1=Q1+ROTJ*EX*FVUP*HCKT*A11
20  J=J+ROTJ*EX
      DERIV(1)=DERIV(1)-Q1*DERIV(2)/Q/J*(2)*CON1
      DERIV(2)=DERIV(2)*CON1/Q
      DERIV(3)=1.0
30  RETURN
      END

```

1 SUBROUTINE REGRES

2 PURPOSE-

3 MAKE A MULTIPLE LINEAR REGRESSION FIT TO DATA WITH A SPECIFIED  
4 FUNCTION WHICH IS LINEAR IN COEFFICIENTS

5

6 CALL REGRES(X,Y,SIGMA,NPTS,INTERMS,I,MODE,YFIT,AJ,A,SIGMA)  
7 SIGMAA,R,RMUL,CHISQ,FTST)

8

9 DESCRIPTION OF PARAMETERS

10 X - ARRAY OF DATA POINTS FOR INDEPENDENT VARIABLE  
11 Y - ARRAY OF DATA POINTS FOR DEPENDENT VARIABLE

12 SIGMA - ARRAY OF STANDARD DEVIATIONS FOR Y DATA POINTS

13 NPTS - NUMBER OF PAIRS OF DATA POINTS

14 INTERMS - NUMBER OF COEFFICIENTS

15 I - A PARAMETER FOR USE IN FCN

16 MODE - DETERMINES METHOD OF WEIGHTING LEAST-SQUARES FIT

17 +1 (INSTRUMENTAL) WEIGHT(I) = 1./SIGMA\*\*2

18 0 (NO WEIGHTING) WEIGHT(I) = 1.

19 -1 (STATISTICAL) WEIGHT(I) = 1./Y(I)

20 YFIT - ARRAY OF CALCULATED VALUES OF Y

21 AJ - CONSTANT TERM

22 A - ARRAY

23 SIGMA0 - STANDARD DEVIATION OF AJ

24 SIGMAA - ARRAY OF STANDARD DEVIATIONS FOR COEFFICIENTS

25 R - ARRAY OF LINEAR CORRELATION COEFFICIENTS

26 RMUL - MULTIPLE LINEAR CORRELATION COEFFICIENTS

27 CHISQ - REDUCED CHI SQUARE FOR THE FIT

28 FTST - VALUE OF F FOR TEST OF FIT

29 SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED

30 FNC(X,I,J,I)

31 EVALUATES THE FUNCTION FOR THE JTH TERM AND ITH DATA POINT

32 AND I IS A PARAMETER FOR USE IN FNC

33 MATINV(INTERMS,DET)

34 INVERTS A SYMMETRIC TWO-DIMENSIONAL MATRIX OF ORDER INTERMS

35 AND CALCULATES ITS DETERMINANT

36 COMMENTS

37 THIS PROGRAM IS A SLIGHTLY MODIFIED VERSION OF ONE APPEARING IN  
38 BEVINGTON. DIMENSION STATEMENTS ARE VALID FOR NPTS UP TO 100  
39 AND INTERMS UP TO 40.

40 VERSION 12-10-77-1

41 DEC. 10, 1977

42 J. J. C. S. P. H. J. K.

43 SUBROUTINE REGRES(X,Y,SIGMA,NPTS,INTERMS,I,MODE,YFIT,AJ,A,SIGMA),S

44 SIGMAA,R,RMUL,CHISQ,FTST)

45 DOUBLE PRECISION ARRAY,SUM,YMEAN,SIGMA,CHISQ,XMEAN,SIGMAX

46 DOUBLE PRECISION FCN

47 COMMON/Z/NUP,ISSP,IAFN,NTP,IDLITAV,IFAB

48 COMMON/W/ME,MEXE,MEYC,MEZE,WEA,MLE,SEBL,AE,GE,JC,QUE,JRE,PL,MESENE

49 COMMON/AA/ARAY(40,40)

50 COMMON/FF/FCFN(100,40)

51 DIMENSION X(1),Y(1),SIGMA(1),YFIT(1),A(1),SIGMAA(1),R(1)

52 DIMENSION WEIGHT(100),XMEAN(40),SIGMAX(40)

53 INITIALIZE SUMS AND ARRAYS

```

00      SUM=Y*LAN=SIGMA=CHISQ=0.000
      RMUL=0.0
      DO 17 I=1,NPTS
17      YFIT(I)=0.0
      DO 25 J=1,NTERMS
      XMEAN(J)=SIGMA(J)=0.000
      R(J)=A(J)=SIGMA(J)=0.0
      DO 25 K=1,NTERMS
25      ARRAY(J,K)=0.0
      ACCUMULATE WEIGHTED SUMS
      DO 31 I=1,NPTS
      IF (MOD(I),32,37,33)
32      IF (Y(I)) 35,37,33
33      WEIGHT(I)=1./Y(I)
      DO 37 I=1,NPTS
35      WEIGHT(I)=1./(-Y(I))
      GO TO 41
37      WEIGHT(I)=1.
      GO TO 41
39      WEIGHT(I)=1./SIGMA(I)/SIGMA(I)
41      SUM=SUM+WEIGHT(I)
      YMEAN=YMEAN+WEIGHT(I)*Y(I)
      DO 44 J=1,NTERMS
      FCIN(I,J)=FNV(X,I,J,I)
44      XMEAN(J)=XMEAN(J)+WEIGHT(I)*FCIN(I,J)
50      CONTINUE
      YMEAN=YMEAN/SUM
      DO 53 J=1,NTERMS
53      XMEAN(J)=XMEAN(J)/SUM
      FNPTS=FNPTS
      WMEAN=SUM/FNPTS
      DO 57 I=1,NPTS
57      WEIGHT(I)=WEIGHT(I)/WMEAN
      ACCUMULATE MATRICES R AND ARRAY
      DO 67 I=1,NPTS
      SIGMA=SIGMA+WEIGHT(I)*(Y(I)-YMEAN)*(Y(I)-YMEAN)
      DO 67 J=1,NTERMS
      FCX=FCIN(I,J)-XMEAN(J)
      SIGMAX(J)=SIGMA(J)+WEIGHT(I)*FCX*FCX
      R(J)=R(J)+WEIGHT(I)*FCX*(Y(I)-YMEAN)
      DO 67 K=1,J
      DO 67 K=1,J
67      ARRAY(J,K)=ARRAY(J,K)+WEIGHT(I)*FCX*(FCIN(I,K)-XMEAN(K))
      FREE=NPTS-1
      SIGMA=JSQRT(SIGMA/FREE)
      DO 78 J=1,NTERMS
      SIGMAX(J)=DSQRT(SIGMAX(J)/FREE)
      R(J)=R(J)/(FREE+SIGMAX(J)+SIGMA)
      DO 78 K=1,J
      ARRAY(J,K)=ARRAY(J,K)/(FREE+SIGMAX(J)+SIGMAX(K))
78      ARRAY(K,J)=ARRAY(J,K)
      INVERT SYMMETRIC MATRIX

```

```

110 0      CALL 4ATINV(NI=4MS,DET)
      IF(DET)101,91,101
      91 AU=SIGMA0=RMUL=CHISQ=FT=ST=0.0
      GO TO 150
120 0      CALCULATE COEFFICIENTS, FIT, AND CHI SQUARE
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932 0
933 0
934 0
935 0
936 0
937 0
938 0
939 0
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975 0
976 0
977 0
978 0
979 0
980 0
981 0
982 0
983 0
984 0
985 0
986 0
987 0
988 0
989 0
990 0
991 0
992 0
993 0
994 0
995 0
996 0
997 0
998 0
999 0
1000 0

```



```

06      LX=EXP(-HCKT*FVU)
        GO TO 30
        RUU=M-1
        RUO=RUO+1.
        FVU=FV(VUP,RUP)
        LX=EXP(-HCKT*FVU)
        U=U+(2.*RUP+1.)*-X
        M=M+1+FVU-FV(VLO,RLO)
        CALL ESTZIN(IJELTAV,IJLO,M,1,M,AA,0B)
        FNV=FV/AA*(2.*RUP+1.)*EX*UPASS(IUP,SSP,IAFN,XI,4)
100     CONTINUE
        FNV=FNV/4*COR1
        RETURN
        END
70

```



```

1  SUBROUTINE ESTEIN(IDELTAV,IVLOWER,M,IMHOLD,M,A,B)
2
3  THIS SUBROUTINE CALCULATES THE EINSTEIN 'A' AND 'B' COEFFICIENTS
4  FOR A GIVEN VALUE OF DELTA V, LOWER VIB. LEVEL, AND ROTATIONAL
5  INDEX M. THIS INDEX IS DEFINED BY:
6
7      M = -J'' = -J' - 1      FOR P BRANCH  M=-1,-2,-3...
8
9      1 = J'' + 1 = J'      FOR R BRANCH  M=1,2,3...
10
11  WHERE J'' IS THE LOWER J VALUE AND J' IS THE UPPER. THE PROGRAM
12  CAN BE USED FOR DELTA V=1,2, OR 3 AND LOWER V UP TO 24. HIGHER
13  VALUES OF VLOWER ARE POSSIBLE, BUT ACCURACY BECOMES QUESTIONABLE.
14  THE CALCULATIONS ARE BASED ON THE WORK OF YOUNG AND EAGHUS-J. CHEM
15  PHYS-VOL 44-NO.11(1966).
16
17  DESCRIPTION OF VARIABLES:
18  IDELTAV - DELTA V FOR THE TRANSITION
19  IVLOWER - LOWER VIBRATIONAL QUANTUM NUMBER
20  M - ROTATIONAL INDEX (DEFINED ABOVE)
21  IMHOLD - IF IMHOLD=1, THE PROGRAM ASSUMES VLOWER AND IDELTAV
22  ARE THE SAME AS IN THE PREVIOUS CALL.
23  A - WAVELENGTH OF THE TRANSITION (INPUT BY USER)
24  B - EINSTEIN 'A' COEFFICIENT (OUTPUT)
25  J - EINSTEIN 'J' COEFFICIENT (OUTPUT)
26
27  SUBROUTINES REQUIRED:
28  FUNCTION F(IDELTAV,IVLOWER,M)
29  THIS FUNCTION CALCULATES THE HERMAN-WALLACE FACTORS FOR 30
30  VERSION 01-05-73-1 JAN. 9, 1976 C. JOSEPH, JR.
31
32  DIMENSION R(3),COF(3,*)
33  DATA X(3),Y(3),Z(3),W(3),V(3),U(3),T(3),S(3),R(3),Q(3),P(3),O(3),N(3),M(3),L(3),K(3),J(3),I(3),H(3),G(3),F(3),E(3),D(3),C(3),B(3),A(3)
34  DATA (COF(1,K),K=1,4)/-3.5025E-5,-3.5025E-5,-3.5025E-5,-3.5025E-5/
35  DATA (COF(2,K),K=1,4)/-3.7520E-3,-3.7520E-3,-3.7520E-3,-3.7520E-3/
36  DATA (COF(3,K),K=1,4)/-1.0747E-3,-1.0747E-3,-1.0747E-3,-1.0747E-3/
37
38  CO.A=2+PI**4/3/H      GUNS=1/3/PI/H/C
39  DATA CONA,CONJ/3.130123862E-29,2.002973158E14/
40
41  CALCULATE THE V-DEPENDENT PART OF THE RADIAL MATRIX ELEMENT
42
43  IF (IMHOLD.EQ.1) GO TO 20
44  VL=IVLOWER
45  LU=IDELTAV
46  PROD=1.0
47  JV=LU
48  PROD=PROD*(VL+JV)/DV
49  LU=LU-1
50  IF (LU.EQ.1) GO TO 10
51  JV=IDELTAV
52  VT=COF(1,1)+VL*(COF(1,2)+VL*(COF(1,3)+VL*(COF(1,4)+1.
53  RV=COF(2,1)+RV(LU)*PROD+VT*RV
54  RVA=CONA*RV
55  RVS=RVA*CONJ
56
57  NOW CONSIDER THE ROTATIONAL DEPENDENCE. TWO QUANTITIES N=LUJ ARE

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```

00      IM=H0AL-LONGUN FACTOR AND THE UPPER AND LOWER LEVEL J-GEN-RACLES.
01      DEFINE THE RATIO OF UPPER TO LOWER LEVEL DEGENERACY AS DUL, DEFINE
02      THE RATIO OF H0AL-LONGUN FACTOR TO UPPER LEVEL DEGENERACY AS SU.
03      IT CAN BE SHOWN
04
20      RM2=2*4+1
05      DUL=K42/FLJAT(2*M-1)
06      SU=FLJAT(M)/RM2
07      NOW CONTINUE WITH THE ROTATIONAL DEPENDENCE
08      RMSU=SU*F(10LLTAV,IVL0AK,M)
09      H-LX=204L THE A AND B COEF., A IS IN 1/SEC, B IS IN CM**2/_RG/SEC
10      A=K44*4*M*M*HMSU
11      B=K43*HMSU*DUL
12      RETURN
13      END

```

FUNCTION F(DLTA,IVLOW,JK,M)

THIS FUNCTION CALCULATES THE HERMAN-WALLACE FACTORS FOR CARBON MONOXIDE AS A FUNCTION OF DELTA V, LOWER VIBRATIONAL LEVEL, AND ROTATIONAL INDEX M. THIS INDEX IS DEFINED BY

M = -J'' - J' - 1 FOR P BRANCH  
M = J'' + 1 = J' FOR R BRANCH

WHERE J'' IS THE LOWER J VALUE AND J' IS THE UPPER. THE PROGRAM CAN BE USED FOR DELTA V=1,2, OR 3 AND LOWER VALUES OF VLOWER ARE POSSIBLE, BUT ACCURACY BECOMES QUESTIONABLE. THIS PROGRAM USES THE CONSTANTS FROM STANFORD UNIVERSITY REPORT SU-IR-REPORT 40-922, BY DAVID JAMES BENDER, MARCH 1970. VLOWER 12-10-77-1 DEC. 10, 1977 C. D. JUS-PA, JK.

IMENSION C(3,6,+),K(0),K(3)  
DATA C(1,K,1),K=1,0)/-2.531E-3,-5.509E-3,-8.73E-3,-1.105E-2,-1.0E-2,-1.457E-2/  
DATA C(2,K,1),K=1,0)/+.071E-2,+.215E-2,+.376E-2,+.320E-2,+.2.8J3E-2,+.2.394E-2/  
DATA C(3,K,1),K=1,0)/1.020E-1,9.234E-2,+.340E-2,+.204E-2,+.074E-2,+.0.191E-2/  
DATA C(1,K,2),K=1,0)/7.010E-4,+.006J0E-4,+.331E-4,+.2.750E-4,+.3.139E-4,+.3.192E-4/  
DATA C(2,K,2),K=1,0)/3.104E-3,+.3.00E-3,+.2.420E-3,+.2.617E-3,+.2.710E-3,+.2.510E-3/  
DATA C(3,K,2),K=1,0)/7.912E-3,+.7.257E-3,+.0.700E-3,+.0.37E-3,+.0.23E-3,+.0.300E-3/  
DATA C(1,K,3),K=1,0)/-2.096E-5,-3.100E-5,-3.350E-5,-3.972E-5,+.2E-5,+.250E-5/  
DATA C(2,K,3),K=1,0)/7.340E-5,+.977E-5,+.0.00E-5,+.2.710E-5,+.0.279E-5,+.1.333E-5/  
DATA C(3,K,3),K=1,0)/+.500E-4,+.3.361E-4,+.3.550E-4,+.0.153E-4,+.2.703E-4,+.2.012E-4/  
DATA C(1,K,4),K=1,0)/1.039E-7,-7.357E-6,-3.312E-7,-7.733E-7,-1.45E-7,-2.20E-6/  
DATA C(2,K,4),K=1,0)/+.395E-5,+.207E-5,+.141E-5,+.3.973E-5,+.3.749E-5,+.3.051E-5/  
DATA C(3,K,4),K=1,0)/2.100E-5,+.2.005E-5,+.1.350E-5,+.1.039E-5,+.0.350E-5,+.1.801E-5/  
DATA K/0.5,+.10,+.10,+.2,+.2+.

THE HERMAN-WALLACE FACTORS CAN BE CALCULATED FOR VLOWER=0,1,2,15, 20,2+. FOR VALUES OF VLOWER DIFFERENT FROM THESE, THE FACTORS ARE CALCULATED USING AN INTERPOLATION/EXTRAPOLATION ROUTINE TAKEN FROM BEVINGTON. NOTE: AFTER TRYING MANY DIFFERENT INTERPOLATION SCHEMES, LINEAR WAS CHOSEN.

NTMS=2  
IV=IVLOWER  
KIN=IV  
K4=4  
K4=K4/10.

FUNCTION F

7-77+ OPT=2

FIN ++0+40

05/10/75 15.00.32

Page-

```

DO 3 J=1,0
  K(J)=1.0+XM*(C(ID,J,1)+XM*(C(ID,J,2)+XM*(C(ID,J,3)+XM*(C(ID,J,4))))
  DO 19 I=1,0
    IF(XIN-X(I))15,17,19
  13 I1=I-1
    GO TO 21
  17 YOUT=X(I)
    GO TO 30
  19 CONTINUE
  I1=5
  I2=I1+1
  21 YOUT=(X(I1)+(XIN-X(I1)))/(X(I2)-X(I1))*(X(I2)-X(I1))
  30 F=YOUT
  RETURN
  END

```

00

05

70



FUNCTION F

7-77+ OPT=2

FIN +.5+440

05/10/75 15.32

440-

```

DO 3 J=1,5
  R(J)=1.0+XM*(C(ID,J,1)+XM*(C(ID,J,2)+XM*(C(ID,J,3)+XM*(C(ID,J,4))))
DO 13 I=1,5
  IF(XIN-X(I))13,17,19
13 I1=I-1
   GO TO 21
17 YOUT=R(I)
   GO TO 30
19 CONTINUE
   I1=5
21 I2=I1+1
   YOUT=R(I1)+(XIN-X(I1))/(X(I2)-X(I1))*(R(I2)-R(I1))
80 F=YOUT
   RETURN
END

```

00

05

70

APPENDIX III

```

1      C      PROGRAM TRACEK(INPUT,OUTPUT)
2      C
3      C      THE PURPOSE OF THIS PROGRAM IS TO CALCULATE THE PARTIAL PRESSURES
4      C      OF VARIOUS INFRARED ABSORBING SPECIES SEEN IN CO2 LASER GAS MIXES.
5      C      THE PROGRAM IS FOR USE WITH THE AFAPL/PND FOURIER TRANSFORM
6      C      SPECTROMETER AND LONG PATH ABSORPTION CELL. THE INPUT DATA
7      C      INCLUDES INTERFEROMETER PARAMETERS, MOLECULAR WEIGHT OF THE ABSORB-
8      C      ING SPECIES, LINE STRENGTH, VARIOUS BROADENING COEFFICIENTS FOR
9      C      THE LINE, PARTIAL PRESSURES OF THE MAJOR SPECIES IN THE GAS, AND
10     C      THE MEASURED PEAK TRANSMITTANCE OF THE LINE. VOIGT PROFILES ARE
11     C      ASSUMED FOR THE ABSORBING LINES.
12     C
13     C      SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
14     C      SUBROUTINE SEEKRLNDP,SSP,IAFN,W0,S,DM4,FGM4,SLFB,I,PP)
15     C      CALCULATES PARTIAL PRESSURE OF THE ABSORBING SPECIES
16     C      SUBROUTINE FOLDLNDP,SSP,IAFN,W0,M,S,DM4,PRHM,PGAS,PLNGTH,T)
17     C      FOLDS AN FTS BANDPASS FUNCTION WITH AN EXPONENTIAL OF A VOIGT
18     C      PROFILE.
19     C      FUNCTION VOIGT(X,Y)
20     C      CALCULATES A VOIGT PROFILE
21     C      FUNCTION RPASSLNDP,SSP,IAFN,VNUO,VNUJ)
22     C      CALCULATES A NORMALIZED BANDPASS FUNCTION FOR AN INTERFEROMETER
23     C
24     C      WITH THE EXCEPTION OF THE FIRST CARD, ALL CARDS ARE READ IN
25     C      THE LIST DIRECTED READ FORMAT OF THE CDC500
26     C
27     C      DATA CARDS
28     C      FIRST CARD - COLUMNS 1-60 FOR A TITLE
29     C      SECOND CARD - INTERFEROMETER PARAMETERS
30     C      1ST NUMBER - NUMBER OF DATA POINTS TAKEN BY THE
31     C      SPECTROMETER
32     C      2ND NUMBER - SAMPLE SPACING OF DATA POINTS IN HALF-
33     C      WAVELENGTHS OF THE HE-NE LASER
34     C      3RD NUMBER - MOLLERITH CHARACTERS DESCRIBING APOD-
35     C      IZATION FUNCTION
36     C      "BX" - BOXCAR APOD.
37     C      "TI" - TRIANGULAR APOD.
38     C      "HG" - HAPF-GENZEL APOD.
39     C
40     C      THIRD CARD - PARTIAL PRESSURES OF THE MAJOR SPECIES (TORR)
41     C      1ST NUMBER - PARTIAL PRESSURE OF CO2
42     C      2ND NUMBER - PARTIAL PRESSURE OF N2
43     C      3RD NUMBER - PARTIAL PRESSURE OF HE
44     C      FOURTH CARD - COMPLETE DESCRIPTION OF THE ABSORBING LINE
45     C      1ST NUMBER - UP TO FIVE MOLLERITH CHARACTERS TO
46     C      NAME THE ABSORBING SPECIES
47     C      2ND NUMBER - THE MOLECULAR (OR ATOMIC) WEIGHT OF
48     C      THE SPECIES
49     C      3RD NUMBER - THE AVE NUMBER OF THE LINE
50     C      4TH NUMBER - THE LINE STRENGTH (CM-2 ATM-1)
51     C      5TH NUMBER - THE SELF BROADENING COEFFICIENT
52     C      (CM-1 ATM-1)
53     C      6TH NUMBER - THE CO2 BROADENING COEF. (CM-1 ATM-1)
54     C      7TH NUMBER - THE N2 BROADENING COEF. (CM-1 ATM-1)
55     C      8TH NUMBER - THE HE BROADENING COEF. (CM-1 ATM-1)
56     C      FIFTH CARD - MEASURED TRANSMITTANCE DATA
57     C      1ST NUMBER - NUMBER OF TRANSMITTANCE MEASUREMENTS
58     C      FOR THE DESCRIBED CONDITIONS

```



SIXTH CARD - CONTROL PARAMETER FOR READING ANOTHER DATA SET  
 (UP TO 10)  
 2ND NUMBER - THIS NUMBER THRU MTH NUMBER ON THE  
 CARD ARE FOR THE TRANSMITTANCE VALUES  
 (PER CENT)  
 THE PARAMETER MAY HAVE THE FOLLOWING VALUES  
 0 - STOP (MUST BE INCLUDED AT SOME POINT)  
 1 - READ A NEW DATA SET STARTING WITH THE THIRD  
 CARD ABOVE AND ENDING WITH ANOTHER CONTROL  
 PARAMETER CARD (4 CARDS)  
 2 - READ A NEW DATA SET STARTING WITH THE 4TH  
 CARD (3 CARDS)  
 3 - READ AN ENTIRE NEW DATA SET STARTING WITH A  
 NEW TITLE CARD

COMMENTS  
 PATHLENGTH IS ASSUMED TO BE 20.25 METERS. TEMPERATURE IS ASSUMED  
 TO BE 296 DEG. K.

VERSION 03-03-80-1 MAR. 03, 1980 C. DEJOSEPH, JR.

DIMENSION TRILIO, TITLE(6)  
 DATA PATH/2025./  
 DATA APR/6.5356625E-10/

READ IN TITLE AND INTERFEROMETER DATA

1-READIO, TITLE(I), I=1,6)  
 10 FORMAT(6A10)  
 READ\*, NDP, SSP, IAFN  
 FNDP=NDP

PRINT TITLE, INTERFEROMETER DATA, AND HEADERS

PRINT30, (TITLE(I), I=1,6)  
 30 FORMAT(1H1, 6A10)  
 ISSP=SSP

PRINT40, NDP, ISSP, IAFN  
 40 FORMAT(1H0, \*INTERFEROMETER PARAMETERS: NDP=\*, 17, 4X, \*SSP=\*, 13, 4X, \*A  
 6FN= \*, 42)

PRINT50  
 50 FORMAT(1H0, \*SPECIES\*, 2X, \*WAVENUM\*, 3X, \*LINE STRENGTH\*, 3X, \*PHE PRES\*,  
 62X, \*N2 PRES\*, 2X, \*C02 PRES\*, 2X, \*SPECIES PRES\*, 2X, \*TOTAL PRES\*, 2X, \*P  
 6, 8, \*H.W.\*, 4X, \*TRANS\*)

PRINT60  
 60 FORMAT(1H1, \*10X, \*(CM-1)\*, 4X, \*(CM-2 ATM-1)\*, 4X, \*(TORR)\*, 3X, \*(TORR)\*,  
 63X, \*(TORR)\*, 6A, \*(TORR)\*, 7X, \*(TORR)\*, 5X, \*(CM-1)\*, 6X, \*(Z)\*)

READ IN DATA

70 READ\*, PC02, PN2, PHE  
 1SK=0

80 READ\*, ISP, WM4, W0, S, BSELF, BCU2, PN2, 4HE  
 READ\*, NT, (TR(I), I=1, NT)

READ\*, IPRIN  
 IF (ISP.EQ.1SK) GO TO 95  
 IF (1SK.EQ.01GO TO 90  
 IF (IC.EQ.1) GO TO 90

```

115 FIC=IC
    PRAV=PREL/FIC
    STGR=SORT((PRELS-FIC*PRAV*PRAV)/(FIC-1.))
    PRINT115,15K,IC,PRAV,STGR
    IF(IIPRIN.EQ.0)STOP
    IF(IIPRIN.EQ.1)GO TO 70
    IF(IIPRIN.EQ.3)GO TO 1
    90 PREL=0.
    PRELS=0.
    IC=0
    125 ISK=ISP
    95 CONTINUE
C
C CALCULATE PARTIAL PRESSURE- GET READY FOR SEEKER1
C
    FGH4=(PC02*8C02*PN2*BN2*PHE*BHE)/760.
    DHW=3.58E-7*SORT(296./MMW)*W0
C*****FINITE APERTURE CORRECTION*****
    APRC=W0*FNDP*APR
    NDP=FNDP/SORT(1+AP2C*APRC)
    135 DO 100 J=1,NT
        TX=TR(J)
        CALL SEEKER1(NDP,SPP,IAFN,W0,S,DHW,FGHW,BSELF,TX,PX)
        PTOT=PX+PC02*PN2*PHE
        PBHW=FGHW*PX*BSELF/760.
        FRAC=PX/PTOT
        PREL=PREL+FRAC
        PRELS=PRELS+FRAC*FRAC
        IC=IC+1
    145 100 PRINT110,ISP,W0,S,PHE,PN2,PC02,PX,PTOT,PBHW,TX
        110 FORMAT(1H,1X,A5.2X,F8.2,5X,1PE10.3,4X,0PF6.1,3X,F6.1,3X,F6.1,5X,1
        6PE9.2,5X,0PF6.1,3X,1PE10.3,2X,0PF7.2)
        115 FORMAT(1H,*,THE AVERAGE RELATIVE CONCENTRATION OF *,A*,
        6*CALCULATED FROM THE ABOVE*,I2,*, MEASUREMENTS IS*,1PE10.3,3X,*STD.
        6 DEV.**,E10.3)
        IF(IIPRIN-1)120,121,118
    150 118 IF(IIPRIN-2)180,80,119
        119 IF(IC-1)1,1,85
        120 IF(IC-1)130,130,85
        121 IF(IC-1)170,70,85
        130 STOP
        END

```